http://www.cas.org/infopolicy.html

=> s l7
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:06:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1806 TO ITERATE

100.0% PROCESSED 1806 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 33571 TO 38669
PROJECTED ANSWERS: 4 TO 200

L9 4 SEA SSS SAM L7

L10 3 L9

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 1.92 21.88

FILE 'REGISTRY' ENTERED AT 14:08:20 ON 25 FEB 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 24 FEB 2008 HIGHEST RN 1005323-41-0
DICTIONARY FILE UPDATES: 24 FEB 2008 HIGHEST RN 1005323-41-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

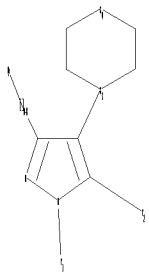
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

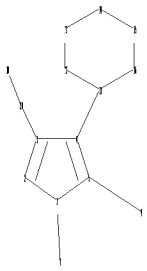
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

10536899

=>
Uploading C:\Documents and Settings\EBernhardt\My
Documents\Stnexp\Queries\10536899.str





chain nodes :
7 9 10 20
ring nodes :
1 2 3 4 5 11 12 13 14 15 16
chain bonds :
1-7 3-20 4-11 5-9 10-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 11-12 11-16 12-13 13-14 14-15 15-16
exact/norm bonds :
1-2 1-5 1-7 2-3 3-4 3-20 4-5 4-11 5-9 10-20
exact bonds :
11-12 11-16 12-13 13-14 14-15 15-16
isolated ring systems :
containing 11 :

G1:H,Ak

G2:C,H

G3:C,N

G4:C,O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 20:CLASS
Generic attributes :
10:
Saturation : Unsaturated

L11 STRUCTURE UPLOADED

=> d l11
L11 HAS NO ANSWERS
L11 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l11
SAMPLE SEARCH INITIATED 14:08:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1655 TO ITERATE

100.0% PROCESSED 1655 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 30660 TO 35540
PROJECTED ANSWERS: 4 TO 200

L12 4 SEA SSS SAM L11

=> s l11 sss full
FULL SEARCH INITIATED 14:08:55 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 31784 TO ITERATE

100.0% PROCESSED 31784 ITERATIONS 135 ANSWERS
SEARCH TIME: 00.00.01

L13 135 SEA SSS FUL L11

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 178.36 200.24

FILE 'CAPLUS' ENTERED AT 14:09:00 ON 25 FEB 2008

FILE COVERS 1907 - 25 Feb 2008 VOL 148 ISS 9
FILE LAST UPDATED: 24 Feb 2008 (20080224/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l13
L14 8 L13

=> d l14 1-8 bib abs hitstr

L14 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:1213121 CAPLUS
DN 147:502389
TI Preparation of diketo-piperazine and piperidine derivatives as antiviral agents
IN Wang, Tao; Kadow, John F.; Zhang, Zhongxing; Yin, Zhiwei; Meanwell, Nicholas A.; Regueiro-Ren, Alicia; Swidorski, Jacob; Han, Ying; Carini, David J.
PA Bristol-Myers Squibb Company, USA
SO U.S. Pat. Appl. Publ., 277pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2007249579	A1	20071025	US 2007-733283	20070410
WO 2007127635	A2	20071108	WO 2007-US66700	20070416

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,

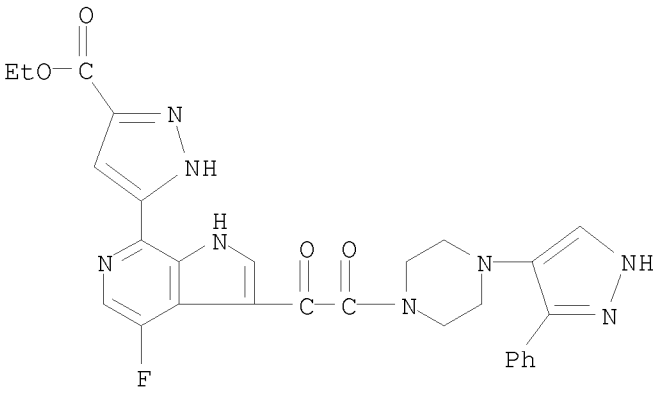
BY, KG, KZ, MD, RU, TJ, TM
PRAI US 2006-794700P P 20060425
US 2006-794703P P 20060425
US 2007-733283 A 20070410
OS MARPAT 147:502389
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

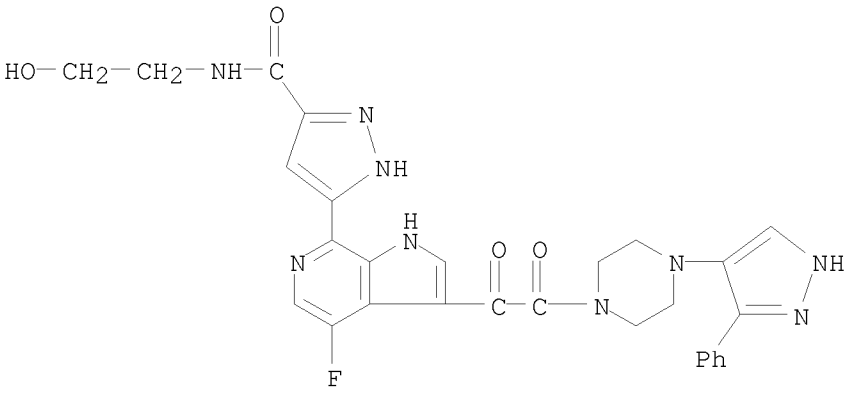
AB Title compds. I [Ring A = (un)substituted 6-membered aryl or nitrogen heteroaryl; R1 = H, alkyl or fluoroalkyl; R2 = H; R3-10 independently = H or (un)substituted alkyl; Y = (un)substituted Ph, monocyclic heteroaryl, bicyclic aryl, etc.; Z = alkyl, alkoxy, cycloalkyl, etc.], and their pharmaceutically acceptable salts, are prepared and disclosed as antiviral agents. Thus, e.g., II was prepared by Friedel-Craft acylation of 7-bromo-4-fluoro-1H-pyrrolo[2,3-c]pyridine with Me chlorooxoacetate followed by amidation with 1-(1-phenyl-1H-tetrazol-5-yl)piperazine (preparation given). In particular, the disclosure is concerned with diketo piperazine and piperidine derivs. that possess unique antiviral activity. EC50 values were determined for I with results reported in ranges with one group possessing EC50 values of ≤ 0.5 μM and the other as > 0.5 μM. More particularly, the present disclosure relates to compds. useful for the treatment of HIV and AIDS.

IT 955046-55-6P 955046-56-7P 955046-57-8P
955046-58-9P 955047-83-3P 955047-84-4P
955047-85-5P 955047-86-6P 955047-87-7P
955047-88-8P 955048-05-2P 955048-12-1P
955048-13-2P 955048-31-4P 955048-32-5P
955049-71-5P 955049-74-8P 955049-76-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diketo-piperazine and piperidine derivs. as antiviral agents)

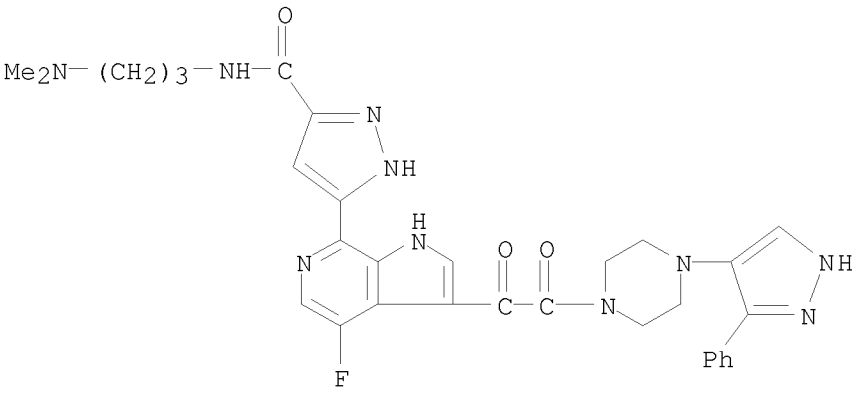
RN 955046-55-6 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 5-[4-fluoro-3-[2-oxo-2-[4-(3-phenyl-1H-pyrazol-4-yl)-1-piperazinyl]acetyl]-1H-pyrrolo[2,3-c]pyridin-7-yl]-, ethyl ester (CA INDEX NAME)



RN 955046-56-7 CAPLUS
CN 1H-Pyrazole-3-carboxamide, 5-[4-fluoro-3-[2-oxo-2-[4-(3-phenyl-1H-pyrazol-4-yl)-1-piperazinyl]acetyl]-1H-pyrrolo[2,3-c]pyridin-7-yl]-N-(2-hydroxyethyl)- (CA INDEX NAME)

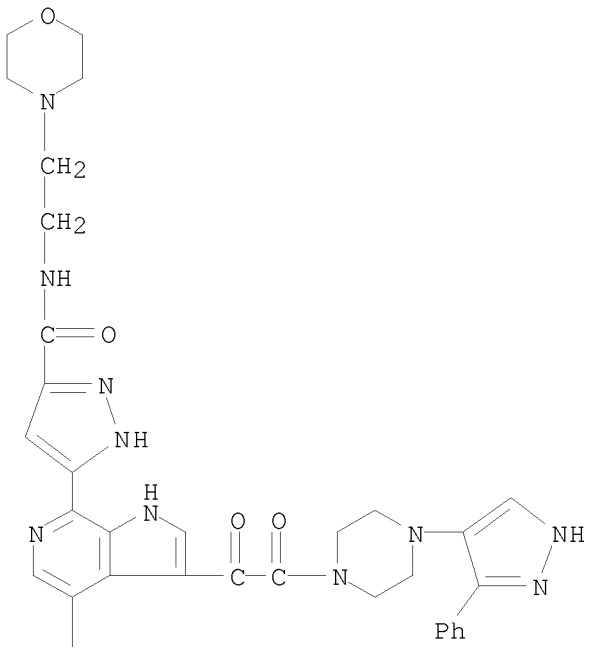


RN 955046-57-8 CAPLUS
CN 1H-Pyrazole-3-carboxamide, N-[3-(dimethylamino)propyl]-5-[4-fluoro-3-[2-oxo-2-[4-(3-phenyl-1H-pyrazol-4-yl)-1-piperazinyl]acetyl]-1H-pyrrolo[2,3-c]pyridin-7-yl]- (CA INDEX NAME)



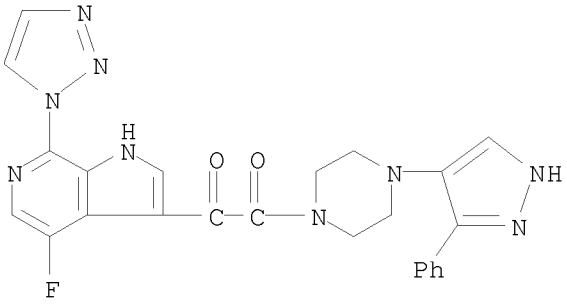
RN 955046-58-9 CAPLUS
CN 1H-Pyrazole-3-carboxamide, 5-[4-fluoro-3-[2-oxo-2-[4-(3-phenyl-1H-pyrazol-4-yl)-1-piperazinyl]acetyl]-1H-pyrrolo[2,3-c]pyridin-7-yl]-N-[2-(4-morpholinyl)ethyl]- (CA INDEX NAME)

PAGE 1-A

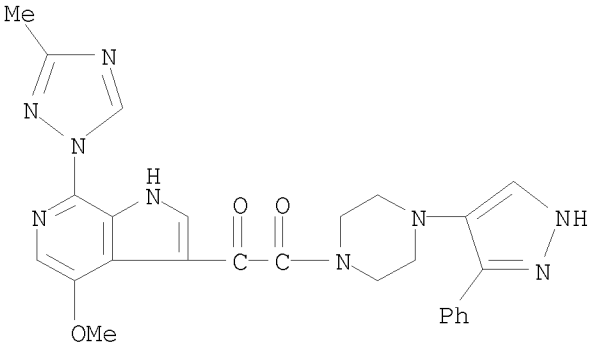


PAGE 2-A

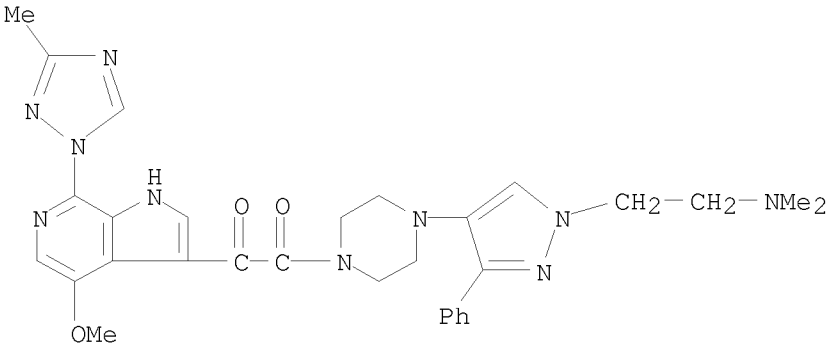
RN 955047-83-3 CAPLUS
CN 1,2-Ethanedione, 1-[4-fluoro-7-(1H-1,2,3-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]-2-[4-(3-phenyl-1H-pyrazol-4-yl)-1-piperazinyl]- (CA INDEX NAME)



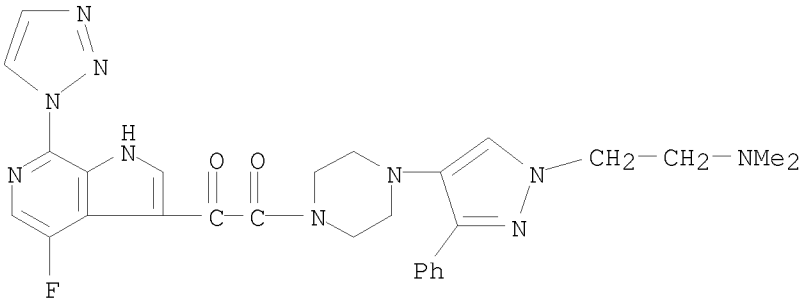
RN 955047-84-4 CAPLUS
CN 1,2-Ethanedione, 1-[4-methoxy-7-(3-methyl-1H-1,2,4-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]-2-[4-(3-phenyl-1H-pyrazol-4-yl)-1-piperazinyl]- (CA INDEX NAME)



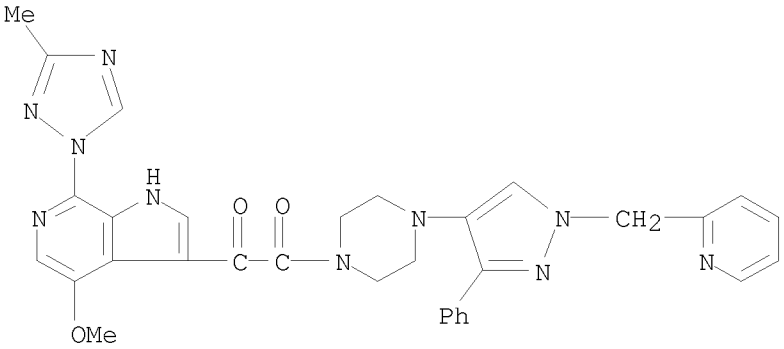
RN 955047-85-5 CAPLUS
CN 1,2-Ethanedione, 1-[4-[1-[2-(dimethylamino)ethyl]-3-phenyl-1H-pyrazol-4-yl]-1-piperazinyl]-2-[4-methoxy-7-(3-methyl-1H-1,2,4-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]- (CA INDEX NAME)



RN 955047-86-6 CAPLUS
CN 1,2-Ethanedione, 1-[4-[1-[2-(dimethylamino)ethyl]-3-phenyl-1H-pyrazol-4-yl]-1-piperazinyl]-2-[4-fluoro-7-(1H-1,2,3-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]- (CA INDEX NAME)

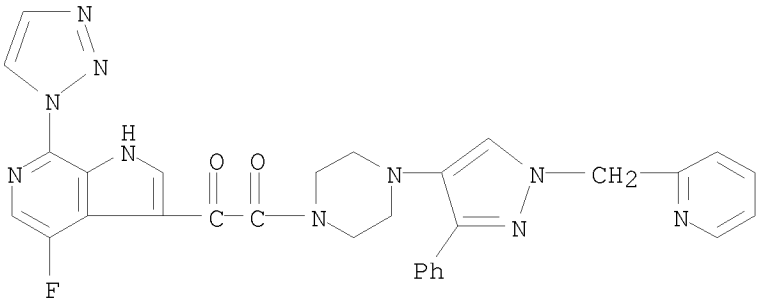


RN 955047-87-7 CAPLUS
CN 1,2-Ethanedione, 1-[4-methoxy-7-(3-methyl-1H-1,2,4-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]-2-[4-[3-phenyl-1-(2-pyridinylmethyl)-1H-pyrazol-4-yl]-1-piperazinyl]- (CA INDEX NAME)

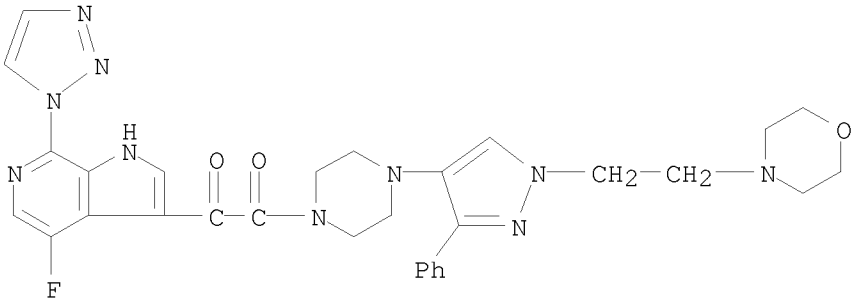


RN 955047-88-8 CAPLUS
CN 1,2-Ethanedione, 1-[4-fluoro-7-(1H-1,2,3-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]-2-[4-[3-phenyl-1-(2-pyridinylmethyl)-1H-pyrazol-4-yl]-1-

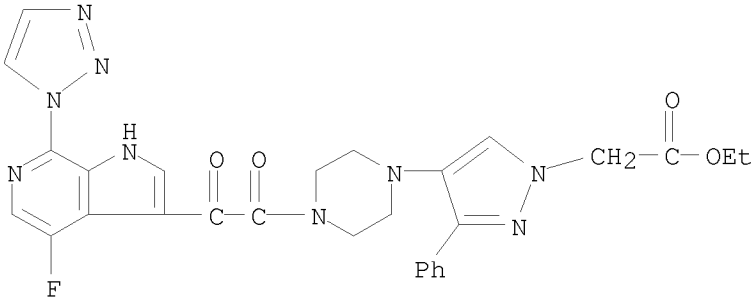
piperazinyl]- (CA INDEX NAME)



RN 955048-05-2 CAPLUS
CN 1,2-Ethanedione, 1-[4-fluoro-7-(1H-1,2,3-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]-2-[4-[1-[2-(4-morpholinyl)ethyl]-3-phenyl-1H-pyrazol-4-yl]-1-piperazinyl]- (CA INDEX NAME)

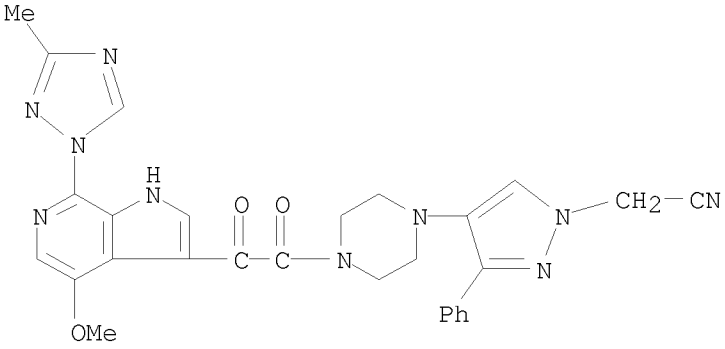


RN 955048-12-1 CAPLUS
CN 1H-Pyrazole-1-acetic acid, 4-[4-[2-[4-fluoro-7-(1H-1,2,3-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]-2-oxoacetyl]-1-piperazinyl]-3-phenyl-, ethyl ester (CA INDEX NAME)

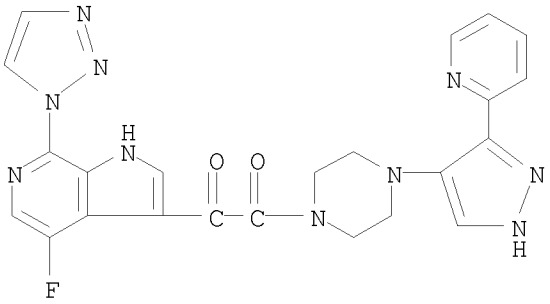


RN 955048-13-2 CAPLUS
CN 1H-Pyrazole-1-acetonitrile, 4-[4-[2-[4-methoxy-7-(3-methyl-1H-1,2,4-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]-2-oxoacetyl]-1-piperazinyl]-3-

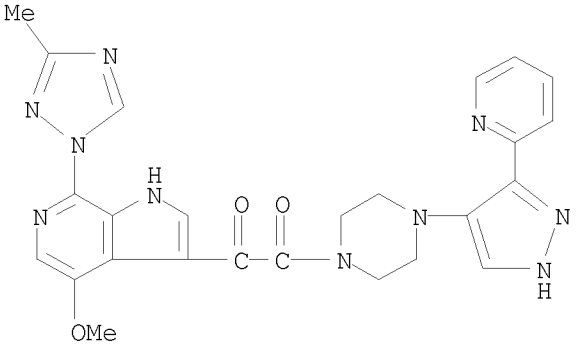
phenyl- (CA INDEX NAME)



RN 955048-31-4 CAPLUS
CN 1,2-Ethanedione, 1-[4-fluoro-7-(1H-1,2,3-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]-2-[4-[3-(2-pyridinyl)-1H-pyrazol-4-yl]-1-piperazinyl]- (CA INDEX NAME)



RN 955048-32-5 CAPLUS
CN 1,2-Ethanedione, 1-[4-methoxy-7-(3-methyl-1H-1,2,4-triazol-1-yl)-1H-pyrrolo[2,3-c]pyridin-3-yl]-2-[4-[3-(2-pyridinyl)-1H-pyrazol-4-yl]-1-piperazinyl]- (CA INDEX NAME)



RN 955049-71-5 CAPLUS

CN 1H-Pyrazole-3-carboxamide, 5-[4-fluoro-3-[2-oxo-2-[4-(3-phenyl-1H-pyrazol-4-yl)-1-piperazinyl]acetyl]-1H-pyrrolo[2,3-c]pyridin-7-yl]-N-(2-hydroxyethyl)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

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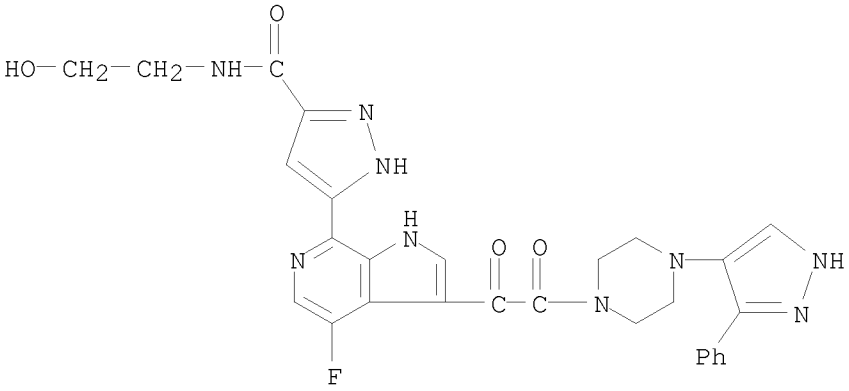
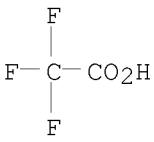
CRN 955046-56-7
CMF C28 H26 F N9 O4



CM 2

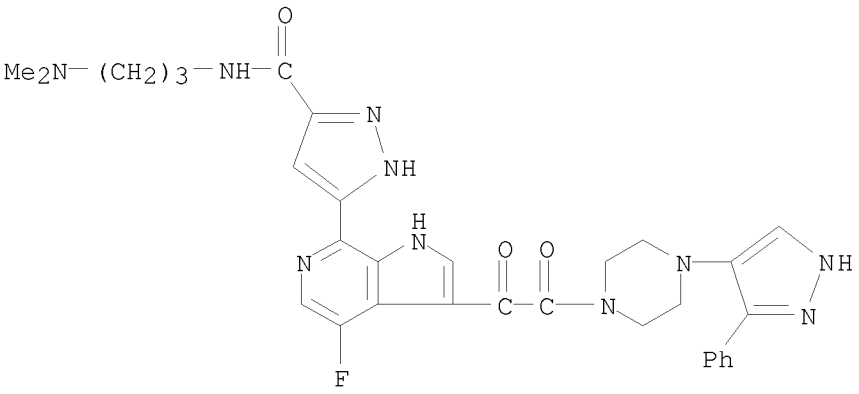
CRN 76-05-1
CMF C2 H F3 O2



RN 955049-74-8 CAPLUS
CN 1H-Pyrazole-3-carboxamide, N-[3-(dimethylamino)propyl]-5-[4-fluoro-3-[2-oxo-2-[4-(3-phenyl-1H-pyrazol-4-yl)-1-piperazinyl]acetyl]-1H-pyrrolo[2,3-c]pyridin-7-yl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

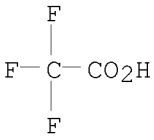
CM 1

CRN 955046-57-8
CMF C31 H33 F N10 O3



CM 2

CRN 76-05-1
CMF C2 H F3 O2

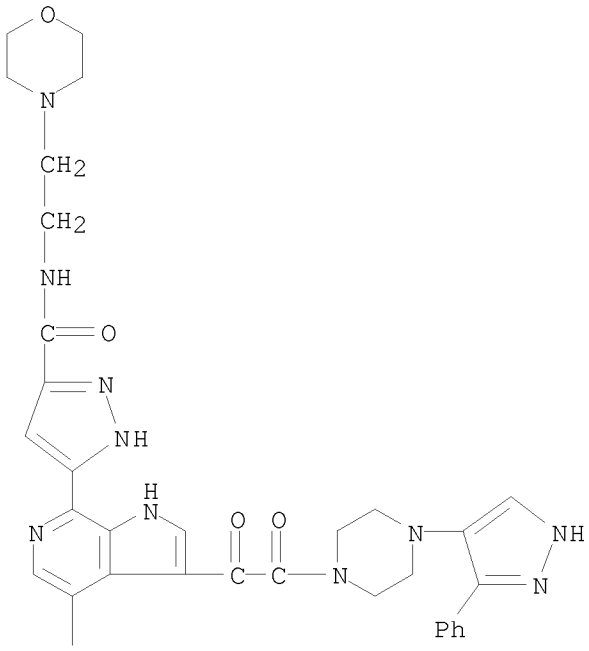


RN 955049-76-0 CAPLUS
CN 1H-Pyrazole-3-carboxamide, 5-[4-fluoro-3-[2-oxo-2-[4-(3-phenyl-1H-pyrazol-4-yl)-1-piperazinyl]acetyl]-1H-pyrrolo[2,3-c]pyridin-7-yl]-N-[2-(4-morpholinyl)ethyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 955046-58-9
CMF C32 H33 F N10 O4

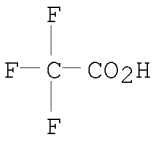
PAGE 1-A



PAGE 2-A

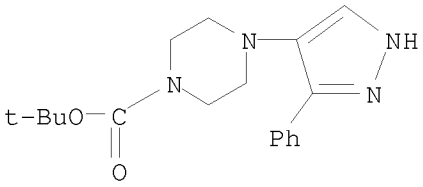
CM 2

CRN 76-05-1
CMF C2 H F3 O2

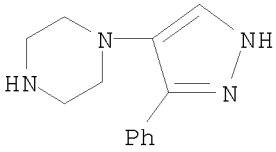


IT 955050-17-6P 955050-18-7P 955050-19-8P
955050-20-1P 955050-21-2P 955050-22-3P
955050-38-1P 955050-39-2P 955050-46-1P
955050-47-2P 955050-48-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of diketo-piperazine and piperidine derivs. as antiviral agents)

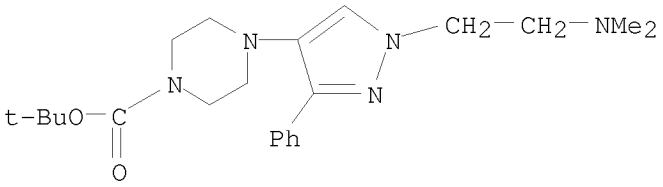
RN 955050-17-6 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-(3-phenyl-1H-pyrazol-4-yl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



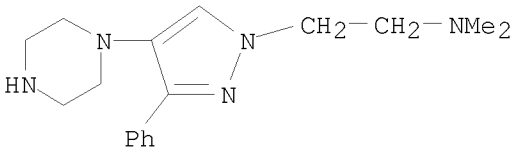
RN 955050-18-7 CAPLUS
CN Piperazine, 1-(3-phenyl-1H-pyrazol-4-yl)- (CA INDEX NAME)



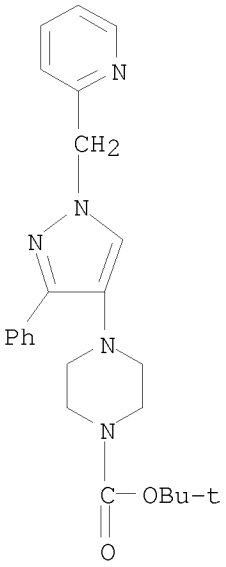
RN 955050-19-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[1-[2-(dimethylamino)ethyl]-3-phenyl-1H-pyrazol-4-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



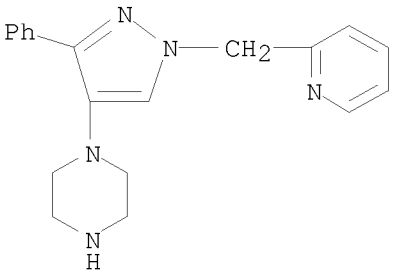
RN 955050-20-1 CAPLUS
CN 1H-Pyrazole-1-ethanamine, N,N-dimethyl-3-phenyl-4-(1-piperazinyl)- (CA INDEX NAME)



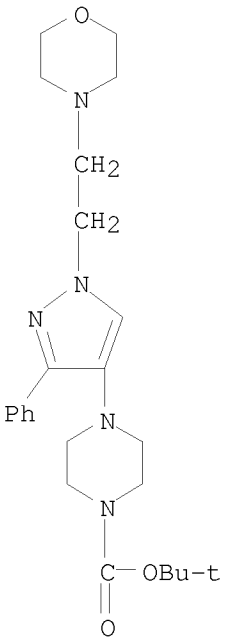
RN 955050-21-2 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[3-phenyl-1-(2-pyridinylmethyl)-1H-pyrazol-4-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



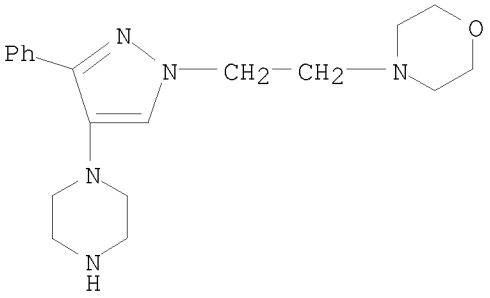
RN 955050-22-3 CAPLUS
CN Piperazine, 1-[3-phenyl-1-(2-pyridinylmethyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)



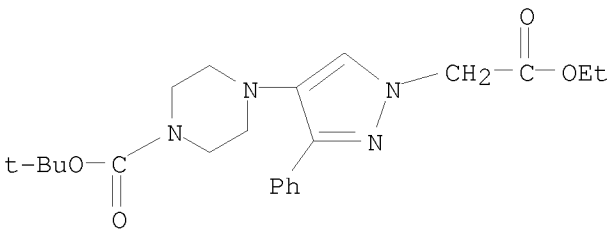
RN 955050-38-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[1-[2-(4-morpholinyl)ethyl]-3-phenyl-1H-pyrazol-4-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



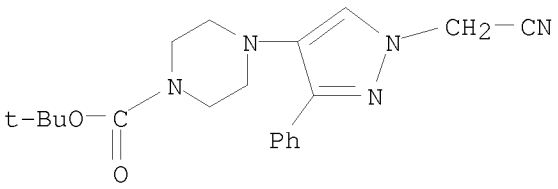
RN 955050-39-2 CAPLUS
CN Morpholine, 4-[2-[3-phenyl-4-(1-piperazinyl)-1H-pyrazol-1-yl]ethyl]- (CA INDEX NAME)



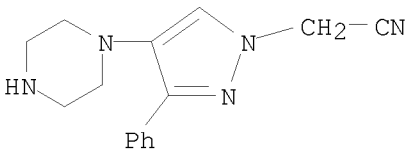
RN 955050-46-1 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[1-(2-ethoxy-2-oxoethyl)-3-phenyl-1H-pyrazol-4-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 955050-47-2 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[1-(cyanomethyl)-3-phenyl-1H-pyrazol-4-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 955050-48-3 CAPLUS
CN 1H-Pyrazole-1-acetonitrile, 3-phenyl-4-(1-piperazinyl)- (CA INDEX NAME)



L14 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:1124920 CAPLUS
DN 145:455028
TI 2-Aminoquinazolin-5-ones and their preparation, pharmaceutical compositions and used in the treatment of cell proliferative diseases
IN Machajewski, Timothy D.; Gao, Zhenhai; Levine, Barry H.; Antonios-McCrea, William; Bellamacina, Cornelia R.; Costales, Abran; Doughan, Brandon M.; Fong, Susan; Hendrickson, Thomas; Lin, Xiaodong; McBride, Christopher; McKenna, Maureen; Rico, Alice C.; Shafer, Cynthia M.; Wang, X. Michael; Zhou, Yasheen; Xia, Yi; Mendenhall, Kris G.
PA Chiron Corporation, USA
SO PCT Int. Appl., 155pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2006113498	A2	20061026	WO 2006-US14194	20060414
WO 2006113498	A3	20070111		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,

KG, KZ, MD, RU, TJ, TM
US 2007027150 A1 20070201 US 2006-404372 20060414
EP 1885701 A2 20080213 EP 2006-750273 20060414
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
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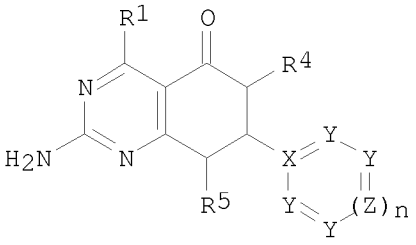
WO 2006-US14194 W 20060414
OS MARPAT 145:455028
GI



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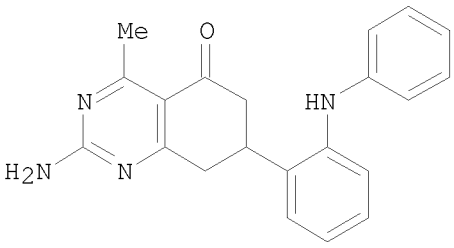


II

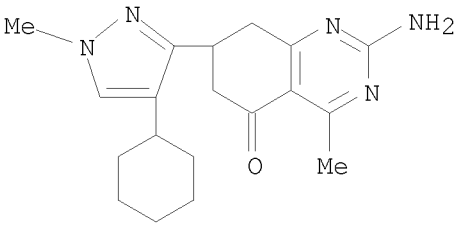
AB 2-Amino-quinazolin-5-one compds. of formula I, stereoisomers, tautomers, pharmaceutically acceptable salts, and prodrugs thereof; compns. that include a pharmaceutically acceptable carrier and one or more of the 2-amino-quinazolin-5-one compds., either alone or in combination with at least one addnl. therapeutic agent. Methods of using the 2-amino-quinazolin-5-one compds. of formula I, either alone or in combination with at least one addnl. therapeutic agent, in the prophylaxis or treatment of cell proliferative diseases. Compds. of formula I wherein n is 0 and 1; when n is 1, X is C, each Y is independently CQ1 and N, and Z is CR2 and N; when n is 0, C is C and N, each Y is independently CQ1, N, NQ2, O and S; Q1 is H, halo, (un)substituted C1-6 alkyl, (un)substituted C2-6 alkenyl, (un)substituted C2-6 alkynyl, (un)substituted C3-7 cycloalkyl, (un)substituted C5-7 cycloalkenyl, (un)substituted (hetero)aryl, (un)substituted amino, CN, NO2 etc.; Q2 is H, (un)substituted C1-6 alkyl, (un)substituted C2-6 alkenyl, (un)substituted C2-6 alkynyl, (un)substituted C3-7 cycloalkyl, (un)substituted C5-7 cycloalkenyl, (un)substituted (hetero)aryl, and (un)substituted heterocyclyl; R1 is H, halo, OH, C1-6 alkoxy, thiol, C1-6 alkylthiol, (un)substituted C1-6 alkyl, amino, alkylamino, arylamino, etc.; R2 is H, halo, (un)substituted C1-6 alkyl, OH and derivs., SH and derivs., and NH2

and derivs.; R4 and R5 are independently H, halo, (un)substituted C1-6 alkyl, OH and derivs., SH and derivs., NH2 and derivs., OCOH and derivs., NHC(O)H and derivs. and NHSO2H and derivs.; and their stereoisomers, tautomers, and pharmaceutically acceptable salts are claimed. Example compound II was prepared by coupling of 2-amino-4-methyl-7-(2-bromophenyl)quinazolin-5-one with aniline. All the invention compds. were evaluated for their HSP90 inhibitory activity. From the assay, it was determined that the some of the compds. exhibited IC50 values less than about 0.1 μM.

IT 913371-99-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of aminoquinazolinone compds. useful in treatment and prophylaxis of cell proliferative diseases)

RN 913371-99-0 CAPLUS

CN 5(6H)-Quinazolinone, 2-amino-7-(4-cyclohexyl-1-methyl-1H-pyrazol-3-yl)-7,8-dihydro-4-methyl- (CA INDEX NAME)



L14 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2006:274325 CAPLUS

DN 144:480380

TI 4-Amino derivatives of the Hsp90 inhibitor CCT018159

AU Barril, Xavier; Beswick, Mandy C.; Collier, Adam; Drysdale, Martin J.; Dymock, Brian W.; Fink, Alexandra; Grant, Kate; Howes, Robert; Jordan, Allan M.; Massey, Andrew; Surgenor, Allan; Wayne, Joanne; Workman, Paul; Wright, Lisa

CS Vernalis Ltd, Cambridge, CB1 6GB, UK

SO Bioorganic & Medicinal Chemistry Letters (2006), 16(9), 2543-2548
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier B.V.

DT Journal

LA English

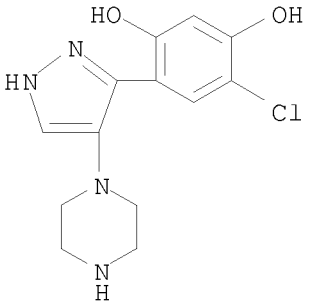
OS CASREACT 144:480380

AB Novel piperazinyl, morpholino and piperidyl derivs. of the pyrazole-based Hsp90 inhibitor CCT018159 are described. Structure-activity relationships have been elucidated by X-ray co-crystal anal. of the new compds. bound to the N-terminal domain of human Hsp90. Key features of the binding mode are essentially identical to the recently reported potent analog VER-49009. The most potent of the new compds. has a methylsulfonylbenzyl substituent appended to the piperazine nitrogen, possesses an IC50 of less than 600 nM binding against the enzyme and demonstrates low micromolar inhibition of tumor cell proliferation.

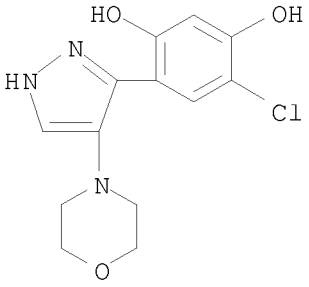
IT 719287-31-7P 719287-32-8P 719287-34-0P
719287-40-8P 719287-51-1P 719287-60-2P

719287-75-9P 719287-76-0P 719287-81-7P
719288-03-6P 719288-04-7P 719288-13-8P
886843-23-8P 886843-24-9P 886843-25-0P
886843-26-1P 886843-27-2P 886843-28-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(amino derivs. of CCT018159 as Hsp90 inhibitors)

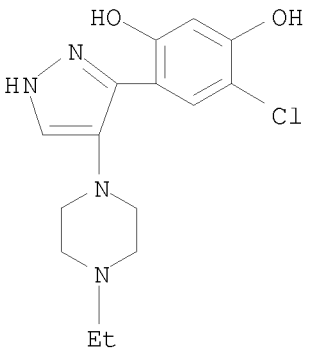
RN 719287-31-7 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



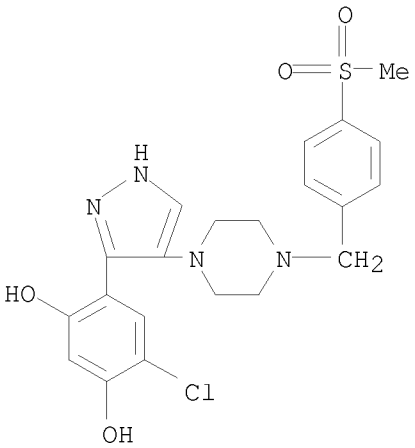
RN 719287-32-8 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-(4-morpholinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



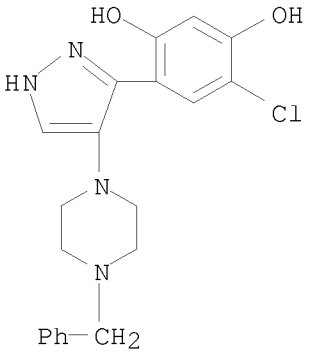
RN 719287-34-0 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-(4-ethyl-1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



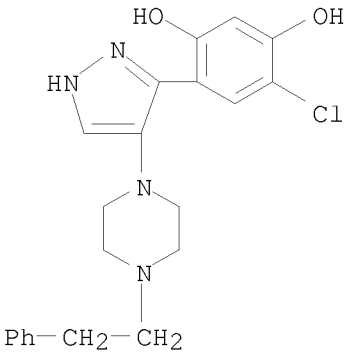
RN 719287-40-8 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-[[4-(methylsulfonyl)phenyl]methyl]-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



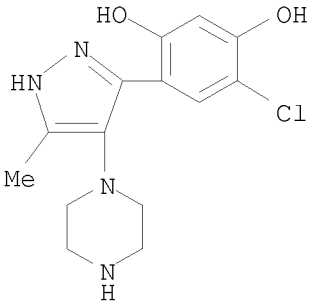
RN 719287-51-1 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-(phenylmethyl)-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



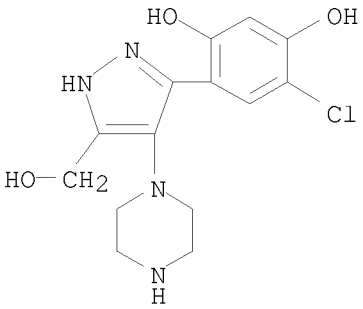
RN 719287-60-2 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-(2-phenylethyl)-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



RN 719287-75-9 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[5-methyl-4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

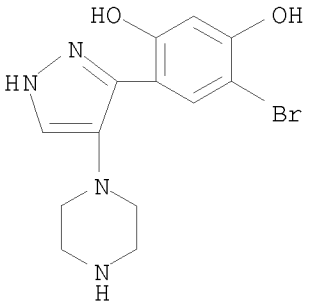


RN 719287-76-0 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[5-(hydroxymethyl)-4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

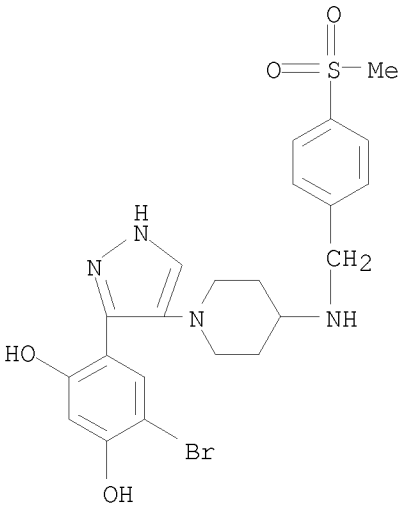


RN 719287-81-7 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX

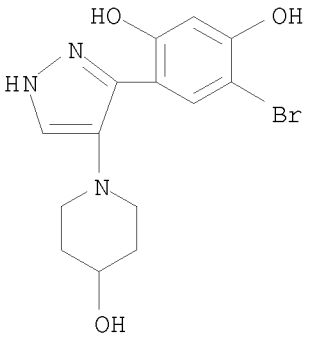
NAME)



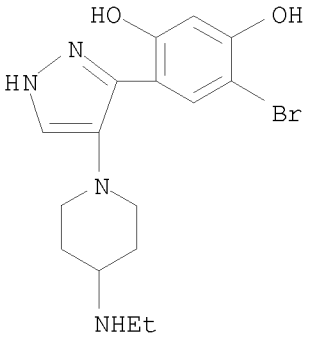
RN 719288-03-6 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-[4-[[[4-(methylsulfonyl)phenyl]methyl]amino]-1-piperidinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



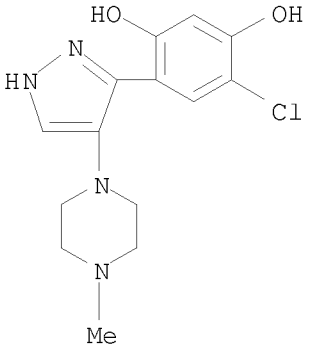
RN 719288-04-7 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-(4-hydroxy-1-piperidinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



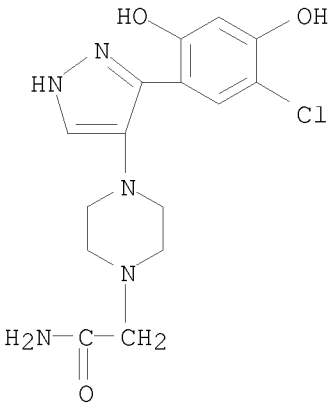
RN 719288-13-8 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-[4-(ethylamino)-1-piperidinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



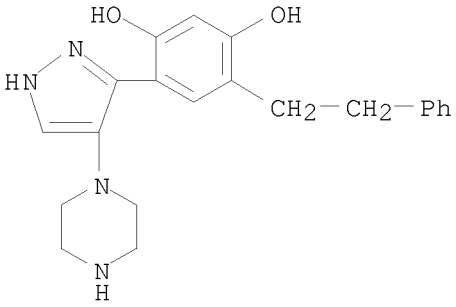
RN 886843-23-8 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-(4-methyl-1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



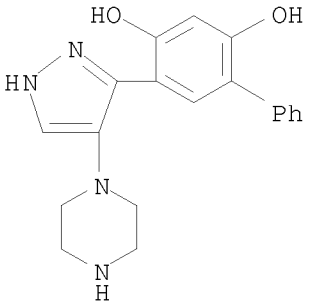
RN 886843-24-9 CAPLUS
CN 1-Piperazineacetamide, 4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)



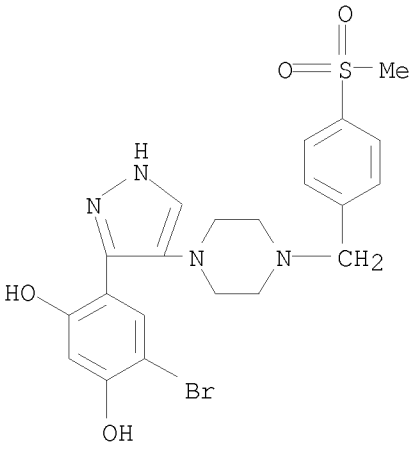
RN 886843-25-0 CAPLUS
CN 1,3-Benzenediol, 4-(2-phenylethyl)-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



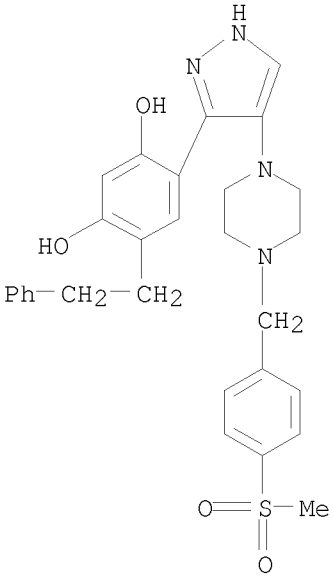
RN 886843-26-1 CAPLUS
CN [1,1'-Biphenyl]-2,4-diol, 5-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



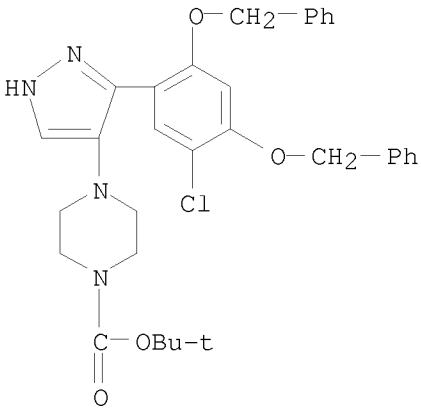
RN 886843-27-2 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-[4-[[4-(methylsulfonyl)phenyl]methyl]-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



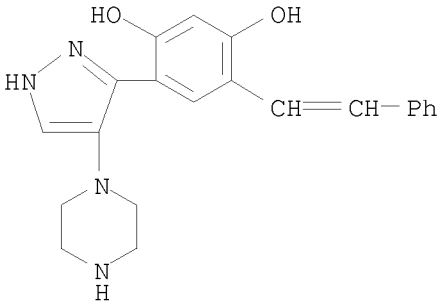
RN 886843-28-3 CAPLUS
CN 1,3-Benzenediol, 4-[4-[4-[[4-(methylsulfonyl)phenyl]methyl]-1-piperazinyl]-1H-pyrazol-3-yl]-6-(2-phenylethyl)- (CA INDEX NAME)



IT 719288-18-3P 886843-31-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(amino derivs. of CCT018159 as Hsp90 inhibitors)
RN 719288-18-3 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[3-[5-chloro-2,4-bis(phenylmethoxy)phenyl]-1H-pyrazol-4-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 886843-31-8 CAPLUS
CN 1,3-Benzenediol, 4-(2-phenylethenyl)-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]-
(CA INDEX NAME)



RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:14363 CAPLUS
DN 142:93425
TI Preparation of N-(cyanomethyl)cycloalkanecarboxamides as cathepsin cysteine protease inhibitors for the treatment of osteoporosis and related diseases
IN Bayly, Christopher; Black, Cameron; Crane, Sheldon; McKay, Daniel J.; Oballa, Renata; Robichaud, Joel
PA Merck Frosst Canada & Co., Can.
SO PCT Int. Appl., 76 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2005000800	A1	20050106	WO 2004-CA948	20040628

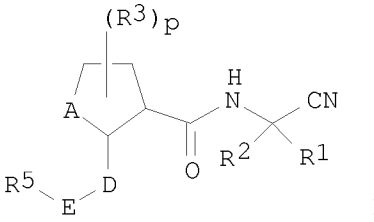
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
SN, TD, TG

	AU 2004251794	A1	20050106	AU 2004-251794	20040628
	CA 2530068	A1	20050106	CA 2004-2530068	20040628
	EP 1644326	A1	20060412	EP 2004-737887	20040628
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	CN 1812967	A	20060802	CN 2004-80018431	20040628
	JP 2007505031	T	20070308	JP 2006-517916	20040628
	US 2007167635	A1	20070719	US 2005-560672	20051214
	IN 2006DN00306	A	20070817	IN 2006-DN306	20060117
PRAI	US 2003-483678P	P	20030630		
	WO 2004-CA948	W	20040628		

OS MARPAT 142:93425

GI



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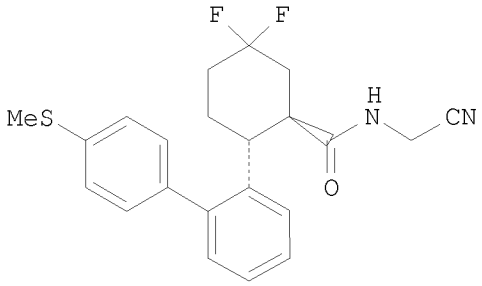
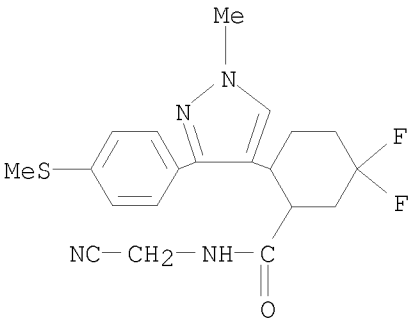


II

AB Title compds. I [wherein R1, R2 = H or (un)substituted alk(en)yl; R1 and R2 can link together; each R3 independently = H, halo or (un)substituted alkyl; two R3 can link together; D = alkyl; D, E = alkenyl, alkynyl, (un)substituted (hetero)aryl, cycloalkyl or heterocyclyl; R5 = H, alk(en/yn)yl, alkoxy, halo, nitro, cyano, (hetero)aryl, cycloalkyl, heterocyclyl or carbonyl, et al.; A = (CH2)n; n = 0-3; p = 0-3, or pharmaceutically acceptable salts, stereoisomers or N-oxide derivs. thereof] were prepared Examples include many N-(cyanomethyl)cyclohexanecarboxamides such as II. The invented compds. are cysteine protease inhibitors, including but not limited to, inhibitors of cathepsin K, L, S and B, with enhanced pharmacol. profiles (not data). Therefore, I and their pharmaceutical compns. are useful for treating diseases in which inhibition of bone resorption is indicated, such as osteoporosis.

IT 819859-25-1P, N-(Cyanomethyl)-5,5-difluoro-2-[1-methyl-3-[4-(methylthio)phenyl]-1H-pyrazol-4-yl]cyclohexanecarboxamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(inhibitor; preparation of (cyanomethyl)cyclohexanecarboxamides as cathepsin cysteine protease inhibitors)
RN 819859-25-1 CAPLUS
CN Cyclohexanecarboxamide, N-(cyanomethyl)-5,5-difluoro-2-[1-methyl-3-[4-(methylthio)phenyl]-1H-pyrazol-4-yl]- (CA INDEX NAME)

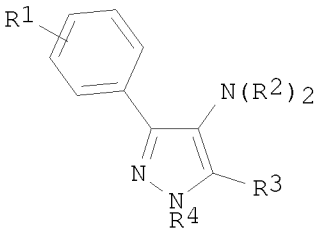


RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:695262 CAPLUS
DN 141:225503
TI Preparation of N,N-disubstituted 4-amino-3(5)-aryl-1(2)H-pyrazoles.
IN Buchs, Jens; Marre, Sabine; Rolfs, Andreas
PA Witega Angewandte Werkstoff-Forschung Gemeinnuetzige G.m.b.H. Adlershof, Germany
SO Ger. Offen., 12 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 10307329	A1	20040826	DE 2003-10307329	20030217
PRAI DE 2003-10307329		20030217		

OS MARPAT 141:225503
GI



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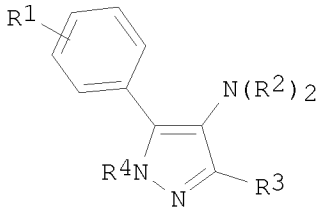


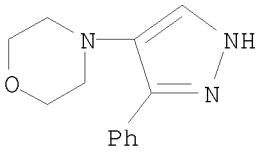
II

AB Title compds. [I, II; R1 = H, halo, MeO, EtO, Mes, CF3, OCF3, OCF2CF3, aryl, NO2, (substituted) amino, morpholino, piperidino, pyrrolidino,

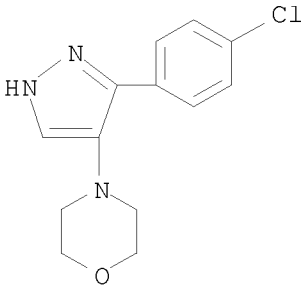
thiomorpholino, etc.; R3 = H, halo, CO2H, cyano, substituted carbonyl, acceptor group, etc.; R4 = H, acyl, (substituted) alkyl], were prepared Thus, Me [N'-(2-morpholino-4-yl-2-thioxo-1-p-tolylethylidene)hydrazino]acetate in HOAc was treated with Br2 followed by 3 h reflux to give 41.3% Me 4-morpholin-4-yl-5--p-tolyl-1(2)H-pyrazole-3-carboxylate.

IT 746662-64-6P 746662-65-7P 746662-67-9P
746662-69-1P 746662-70-4P 746662-72-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(claimed compound; preparation of N,N-disubstituted aminoarylpyrazoles)

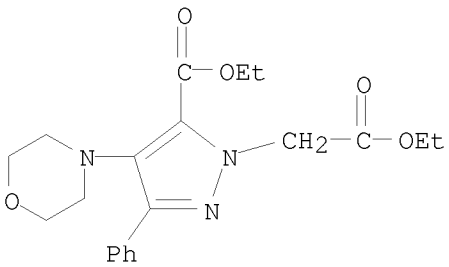
RN 746662-64-6 CAPLUS
CN Morpholine, 4-(3-phenyl-1H-pyrazol-4-yl)- (CA INDEX NAME)



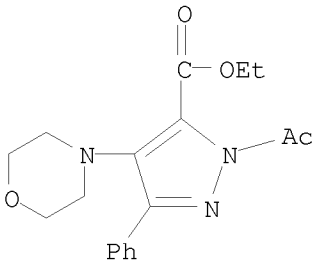
RN 746662-65-7 CAPLUS
CN Morpholine, 4-[3-(4-chlorophenyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)



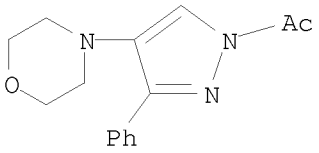
RN 746662-67-9 CAPLUS
CN 1H-Pyrazole-1-acetic acid, 5-(ethoxycarbonyl)-4-(4-morpholinyl)-3-phenyl-, ethyl ester (CA INDEX NAME)



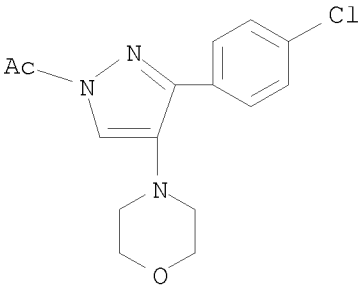
RN 746662-69-1 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-acetyl-4-(4-morpholinyl)-3-phenyl-, ethyl ester (CA INDEX NAME)



RN 746662-70-4 CAPLUS
CN 1H-Pyrazole, 1-acetyl-4-(4-morpholinyl)-3-phenyl- (9CI) (CA INDEX NAME)



RN 746662-72-6 CAPLUS
CN 1H-Pyrazole, 1-acetyl-3-(4-chlorophenyl)-4-(4-morpholinyl)- (9CI) (CA INDEX NAME)



L14 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:546484 CAPLUS
DN 141:106462
TI Preparation of pyrazoles as inhibitors of HSP90
IN Beswick, Mandy Christine; Drysdale, Martin James; Dymock, Brian William; McDonald, Edward
PA Vernalis Cambridge Limited, UK; Cancer Research Technology Ltd.; The Institute of Cancer Research
SO PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004056782	A1	20040708	WO 2003-GB5501	20031218

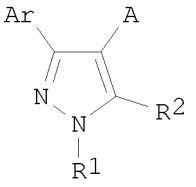
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,

CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2509403	A1	20040708	CA 2003-2509403	20031218
AU 2003292429	A1	20040714	AU 2003-292429	20031218
EP 1572664	A1	20050914	EP 2003-768007	20031218
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003017492	A	20051116	BR 2003-17492	20031218
CN 1738804	A	20060222	CN 2003-80108919	20031218
JP 2006511571	T	20060406	JP 2004-561628	20031218
US 2006148817	A1	20060706	US 2006-536899	20060106
PRAI GB 2002-29618	A	20021219		
WO 2003-GB5501	W	20031218		

OS MARPAT 141:106462

GI



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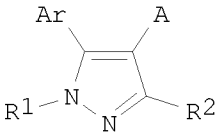


II

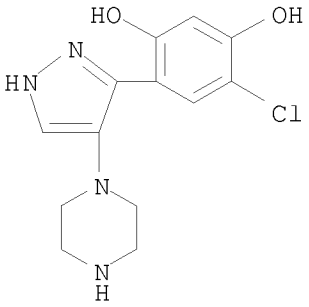
AB The title compds. [I or II; Ar = (un)substituted aryl, arylalkyl, heteroaryl, heteroarylalkyl; R1 = H, alkyl; R2 = H, (un)substituted cycloalkyl, cycloalkenyl, alkyl, alkenyl, alkynyl, carboxyl, carboxamide or carboxyl ester group; A = non-aromatic carbocyclic or heterocyclic ring wherein (i) a ring carbon is optionally substituted, and/or (ii) a ring nitrogen is optionally substituted by a group of formula -(Alk1)p(Cyc)n(Alk3)m(Z)r(Alk2)sQ where Alk1, Alk2 and Alk3 = alkyl; Cyc = carbocyclic or heterocyclic radical; m, n, p, r and s = 0-1; Z = O, S, CO, SO2, etc.; Q = H, (un)substituted carbocyclic or heterocyclic radical] which are inhibitors of HSP90, and are of value in the treatment of diseases responsive to HSP90 inhibition such as cancer, were prepared E.g., a multi-step synthesis of 4-chloro-6-(4-piperazin-1-yl-1H-pyrazol-3-yl)benzene-1,3-diol which showed IC50 of <50 μM in the malachite green ATPase assay, was given.

IT 719287-31-7P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrazoles as inhibitors of HSP90)

RN 719287-31-7 CAPLUS

CN 1,3-Benzenediol, 4-chloro-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA

INDEX NAME)



IT 719287-30-6P 719287-32-8P 719287-33-9P
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719287-40-8P 719287-41-9P 719287-42-0P
719287-43-1P 719287-44-2P 719287-45-3P
719287-46-4P 719287-47-5P 719287-48-6P
719287-49-7P 719287-50-0P 719287-51-1P
719287-52-2P 719287-53-3P 719287-54-4P
719287-55-5P 719287-56-6P 719287-57-7P
719287-58-8P 719287-59-9P 719287-60-2P
719287-61-3P 719287-62-4P 719287-63-5P
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719287-67-9P 719287-68-0P 719287-69-1P
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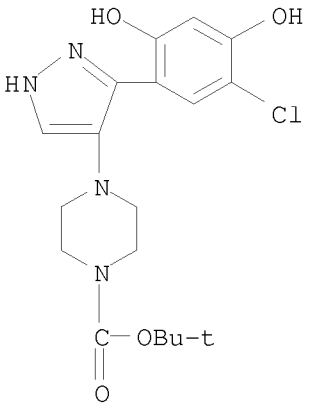
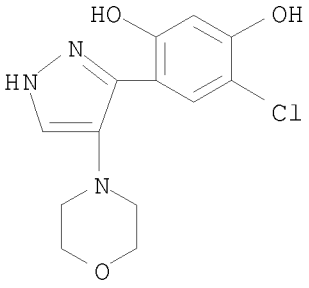
719288-02-5P 719288-03-6P 719288-04-7P
719288-05-8P 719288-06-9P 719288-07-0P
719288-08-1P 719288-09-2P 719288-10-5P
719288-11-6P 719288-12-7P 719288-13-8P
719288-15-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazoles as inhibitors of HSP90)

RN 719287-30-6 CAPLUS

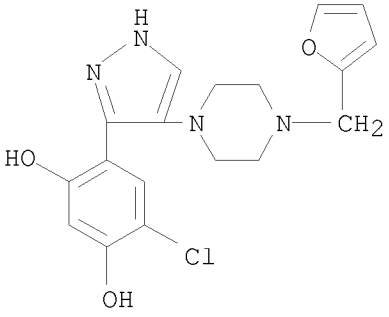
CN 1-Piperazinecarboxylic acid, 4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



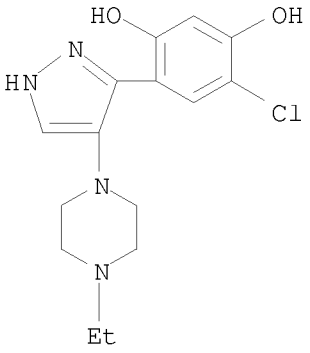
RN 719287-32-8 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-(4-morpholinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



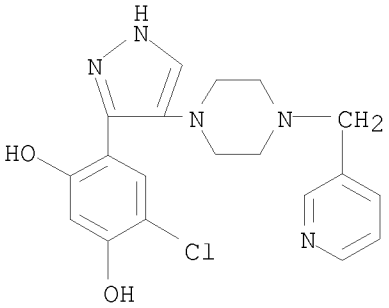
RN 719287-33-9 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-(2-furanylmethyl)-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



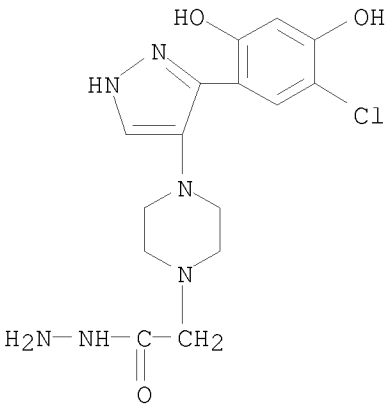
RN 719287-34-0 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-(4-ethyl-1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



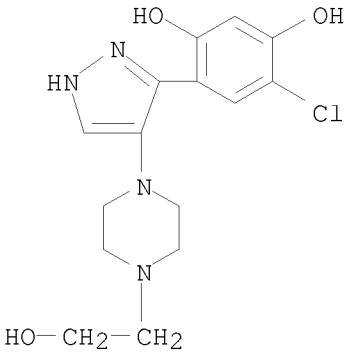
RN 719287-35-1 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-(3-pyridinylmethyl)-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



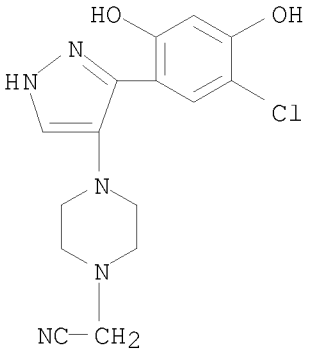
RN 719287-36-2 CAPLUS
CN 1-Piperazineacetic acid, 4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-, hydrazide (CA INDEX NAME)



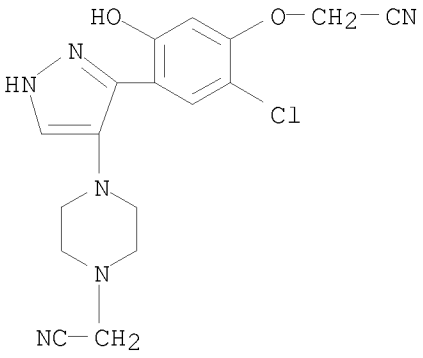
RN 719287-37-3 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-(2-hydroxyethyl)-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



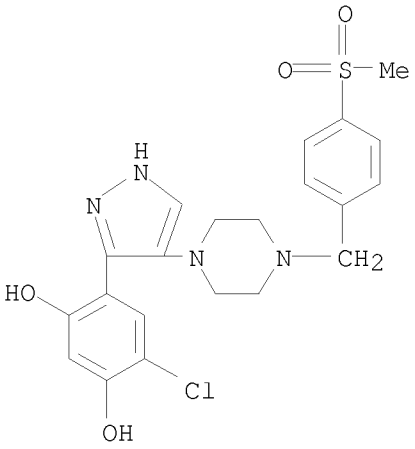
RN 719287-38-4 CAPLUS
CN 1-Piperazineacetonitrile, 4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)



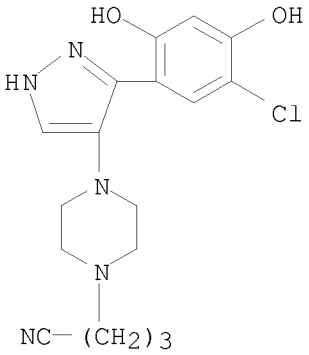
RN 719287-39-5 CAPLUS
CN 1-Piperazineacetonitrile, 4-[3-[5-chloro-4-(cyanomethoxy)-2-hydroxyphenyl]-1H-pyrazol-4-yl]- (CA INDEX NAME)



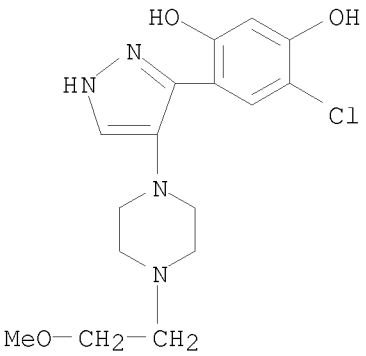
RN 719287-40-8 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-[[4-(methylsulfonyl)phenyl]methyl]-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



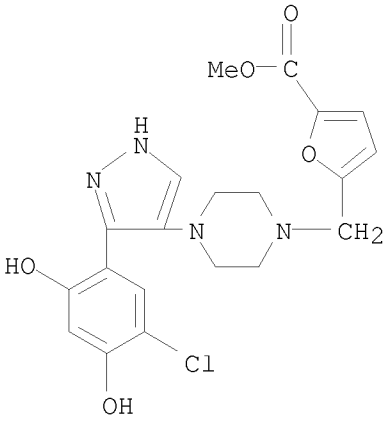
RN 719287-41-9 CAPLUS
CN 1-Piperazinebutanenitrile, 4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)



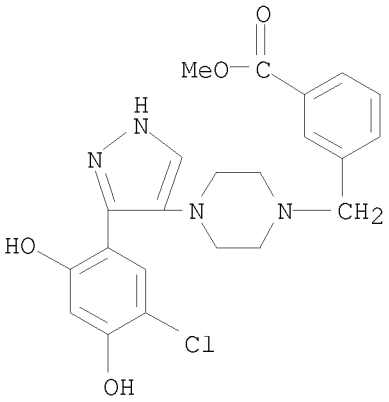
RN 719287-42-0 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-(2-methoxyethyl)-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



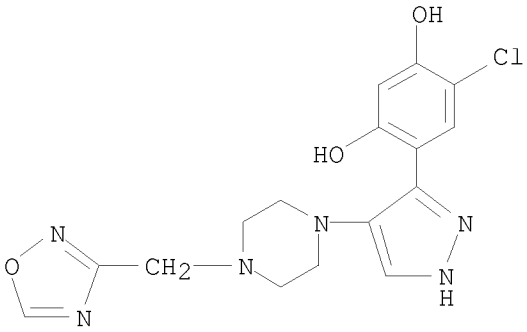
RN 719287-43-1 CAPLUS
CN 2-Furancarboxylic acid, 5-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]methyl]-, methyl ester (CA INDEX NAME)



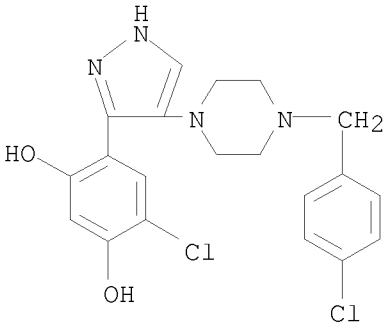
RN 719287-44-2 CAPLUS
CN Benzoic acid, 3-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]methyl]-, methyl ester (CA INDEX NAME)



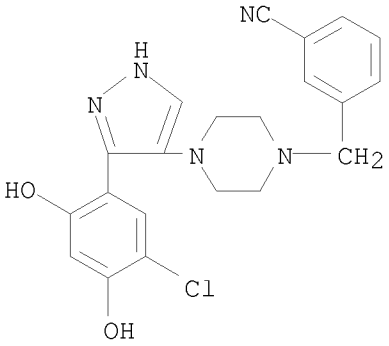
RN 719287-45-3 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-(1,2,4-oxadiazol-3-ylmethyl)-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



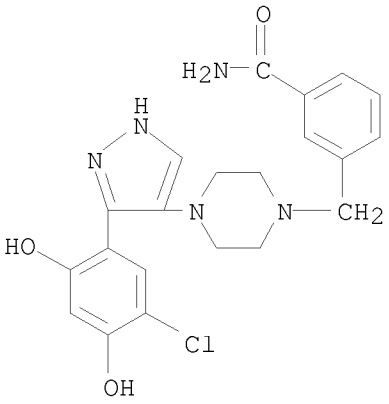
RN 719287-46-4 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-[(4-chlorophenyl)methyl]-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



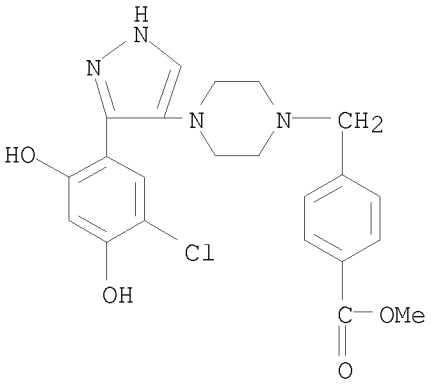
RN 719287-47-5 CAPLUS
CN Benzonitrile, 3-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]methyl]- (CA INDEX NAME)



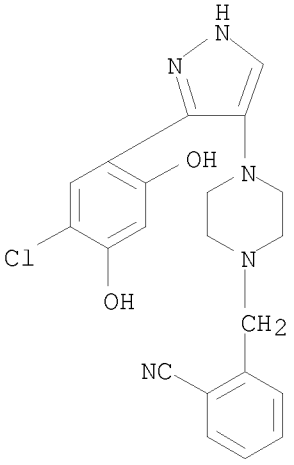
RN 719287-48-6 CAPLUS
CN Benzamide, 3-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]methyl]- (CA INDEX NAME)



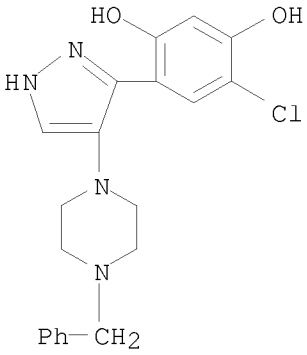
RN 719287-49-7 CAPLUS
CN Benzoic acid, 4-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]methyl]-, methyl ester (CA INDEX NAME)



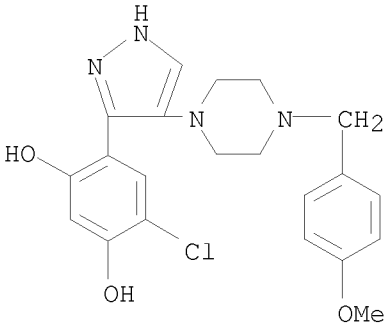
RN 719287-50-0 CAPLUS
CN Benzonitrile, 2-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]methyl]- (CA INDEX NAME)



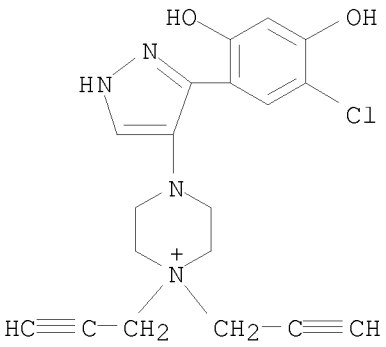
RN 719287-51-1 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-(phenylmethyl)-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



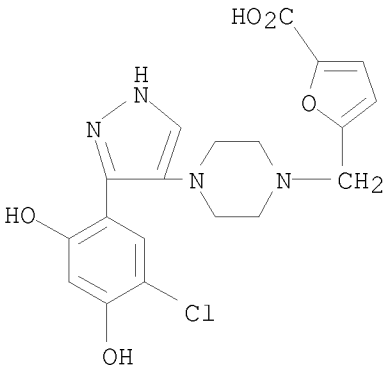
RN 719287-52-2 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-[(4-methoxyphenyl)methyl]-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



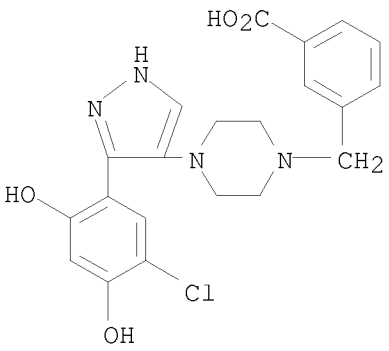
RN 719287-53-3 CAPLUS
CN Piperazinium, 4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1,1-di-2-propynyl- (9CI) (CA INDEX NAME)



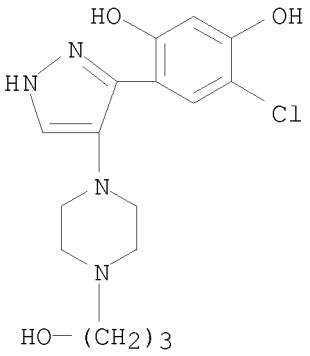
RN 719287-54-4 CAPLUS
CN 2-Furancarboxylic acid, 5-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]methyl]- (CA INDEX NAME)



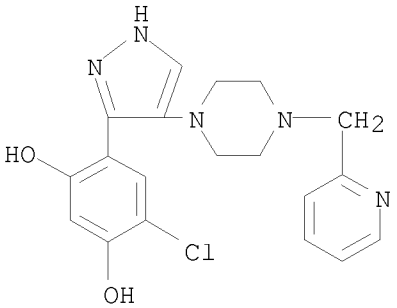
RN 719287-55-5 CAPLUS
CN Benzoic acid, 3-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]methyl]- (CA INDEX NAME)



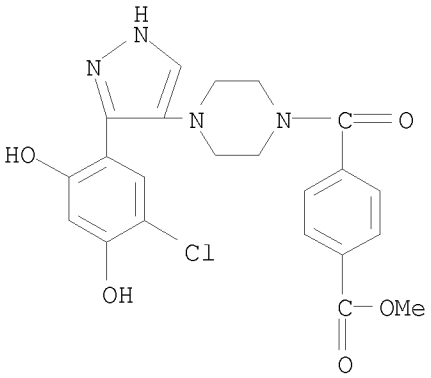
RN 719287-56-6 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-(3-hydroxypropyl)-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



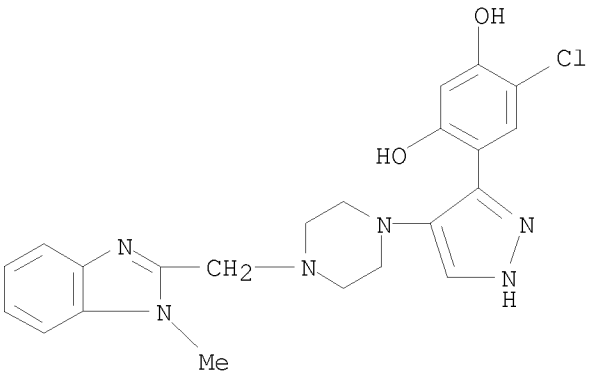
RN 719287-57-7 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-(2-pyridinylmethyl)-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



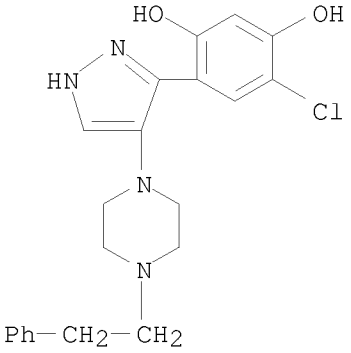
RN 719287-58-8 CAPLUS
CN Benzoic acid, 4-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]carbonyl]-, methyl ester (CA INDEX NAME)



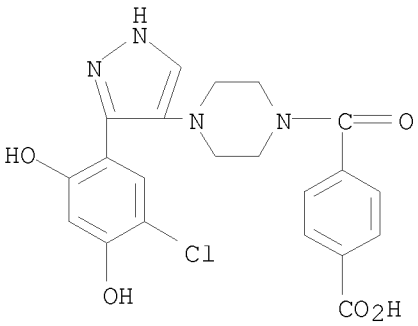
RN 719287-59-9 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-[(1-methyl-1H-benzimidazol-2-yl)methyl]-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



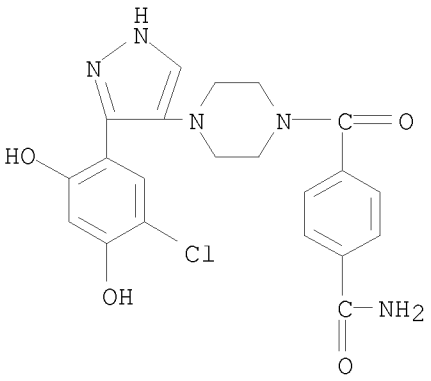
RN 719287-60-2 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-(2-phenylethyl)-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



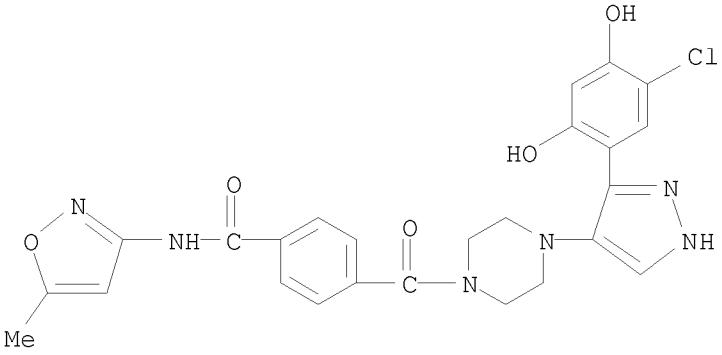
RN 719287-61-3 CAPLUS
CN Benzoic acid, 4-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]carbonyl]- (CA INDEX NAME)



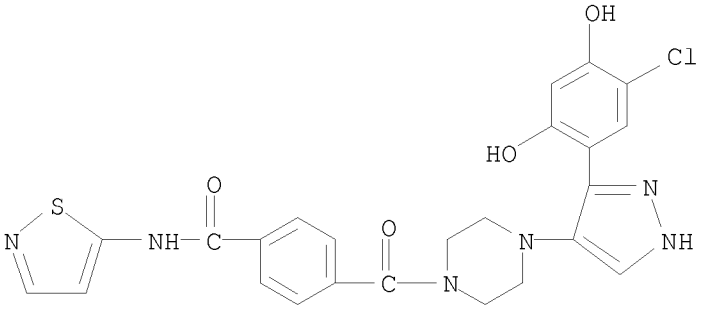
RN 719287-62-4 CAPLUS
CN Benzamide, 4-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]carbonyl]- (CA INDEX NAME)



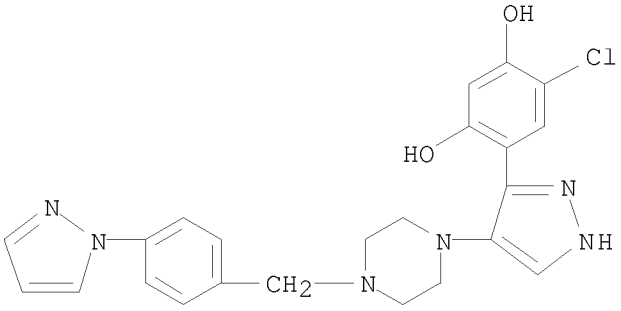
RN 719287-63-5 CAPLUS
CN Benzamide, 4-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]carbonyl]-N-(5-methyl-3-isoxazolyl)- (CA INDEX NAME)



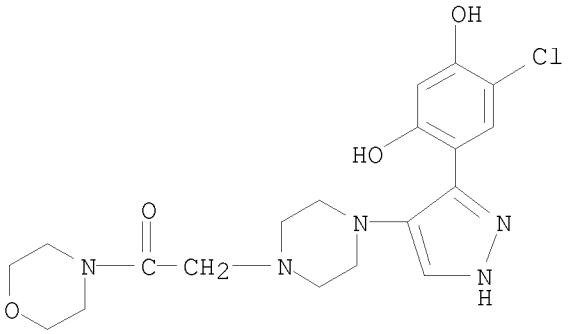
RN 719287-64-6 CAPLUS
CN Benzamide, 4-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]carbonyl]-N-5-isothiazolyl- (CA INDEX NAME)



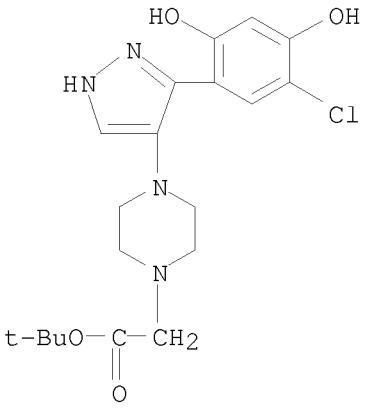
RN 719287-65-7 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-[[4-(1H-pyrazol-1-yl)phenyl]methyl]-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



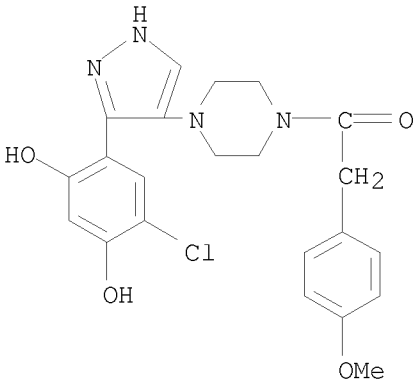
RN 719287-66-8 CAPLUS
CN Morpholine, 4-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]acetyl]- (9CI) (CA INDEX NAME)



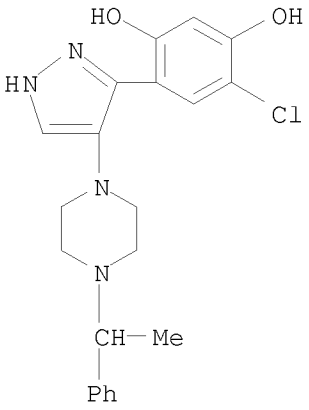
RN 719287-67-9 CAPLUS
CN 1-Piperazineacetic acid, 4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



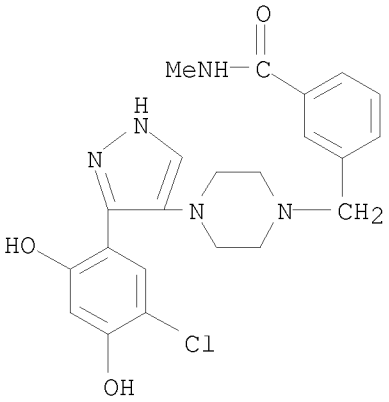
RN 719287-68-0 CAPLUS
CN Piperazine, 1-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-4-[(4-methoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)



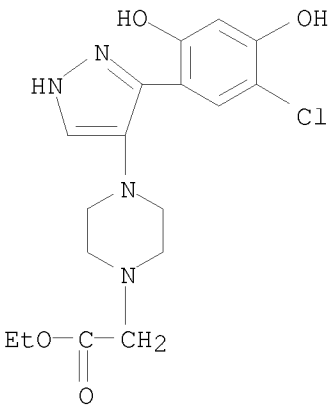
RN 719287-69-1 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[4-[4-(1-phenylethyl)-1-piperazinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



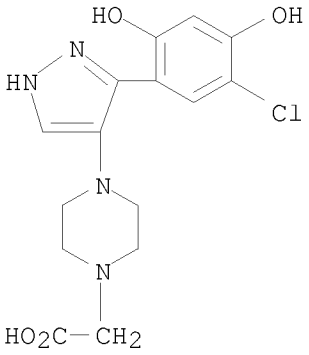
RN 719287-70-4 CAPLUS
CN Benzamide, 3-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]methyl]-N-methyl- (CA INDEX NAME)



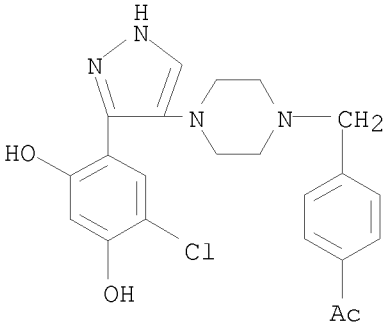
RN 719287-71-5 CAPLUS
CN 1-Piperazineacetic acid, 4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-, ethyl ester (CA INDEX NAME)



RN 719287-72-6 CAPLUS
CN 1-Piperazineacetic acid, 4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)

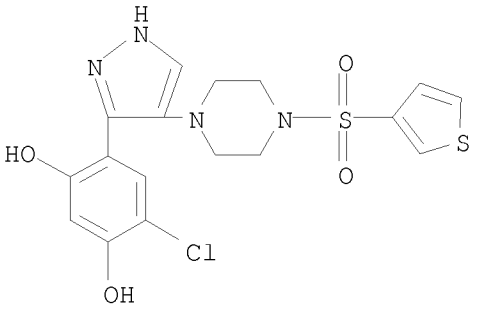


RN 719287-73-7 CAPLUS
CN Ethanone, 1-[4-[[4-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-1-piperazinyl]methyl]phenyl]- (CA INDEX NAME)

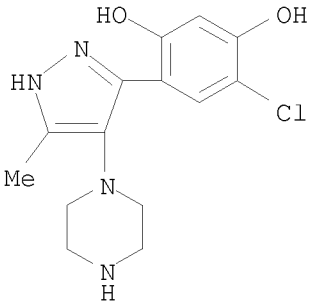


RN 719287-74-8 CAPLUS
CN Piperazine, 1-[3-(5-chloro-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-4-(3-

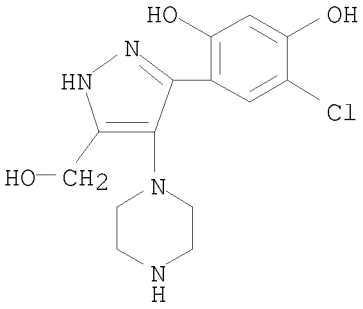
thienylsulfonyl)- (9CI) (CA INDEX NAME)



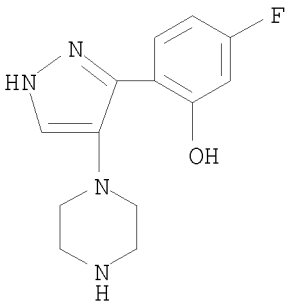
RN 719287-75-9 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[5-methyl-4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



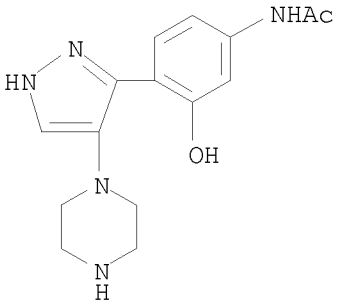
RN 719287-76-0 CAPLUS
CN 1,3-Benzenediol, 4-chloro-6-[5-(hydroxymethyl)-4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



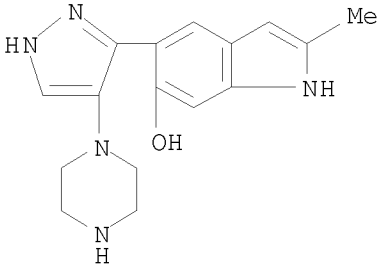
RN 719287-78-2 CAPLUS
CN Phenol, 5-fluoro-2-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



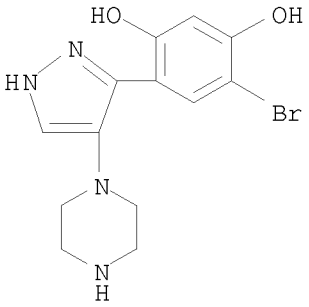
RN 719287-79-3 CAPLUS
CN Acetamide, N-[3-hydroxy-4-[4-(1-piperazinyl)-1H-pyrazol-3-yl]phenyl]- (CA INDEX NAME)



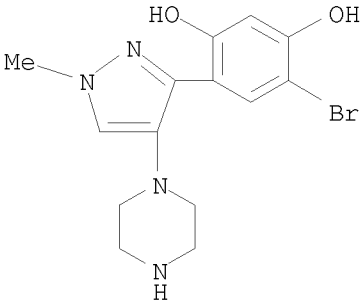
RN 719287-80-6 CAPLUS
CN 1H-Indol-6-ol, 2-methyl-5-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



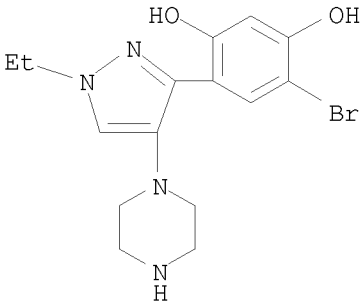
RN 719287-81-7 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



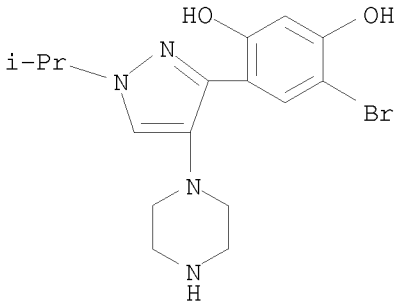
RN 719287-83-9 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[1-methyl-4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



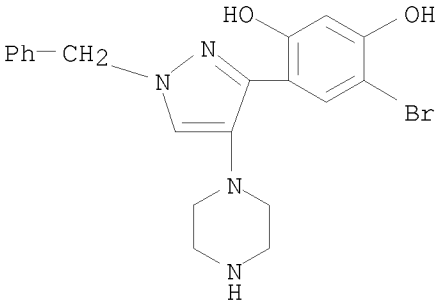
RN 719287-85-1 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[1-ethyl-4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



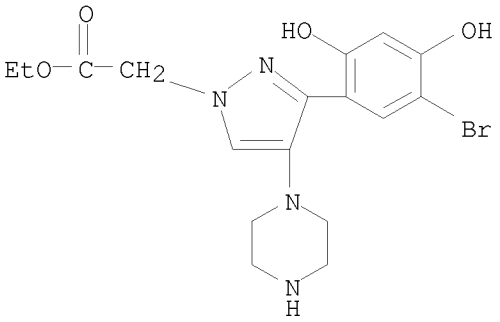
RN 719287-87-3 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[1-(1-methylethyl)-4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



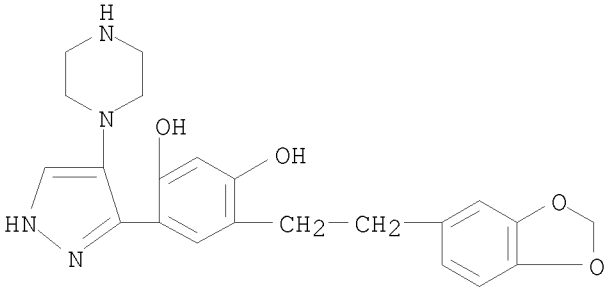
RN 719287-89-5 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[1-(phenylmethyl)-4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



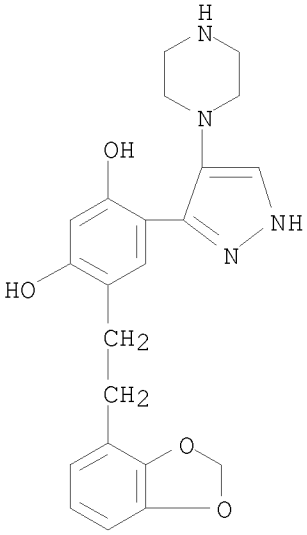
RN 719287-90-8 CAPLUS
CN 1H-Pyrazole-1-acetic acid, 3-(5-bromo-2,4-dihydroxyphenyl)-4-(1-piperazinyl)-, ethyl ester (CA INDEX NAME)



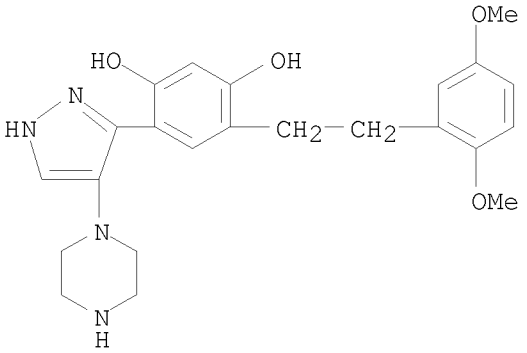
RN 719287-91-9 CAPLUS
CN 1,3-Benzenediol, 4-[2-(1,3-benzodioxol-5-yl)ethyl]-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



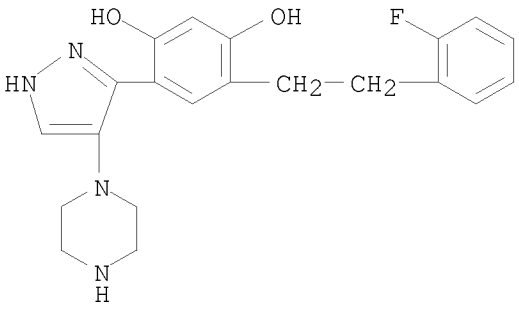
RN 719287-92-0 CAPLUS
CN 1,3-Benzenediol, 4-[2-(1,3-benzodioxol-4-yl)ethyl]-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



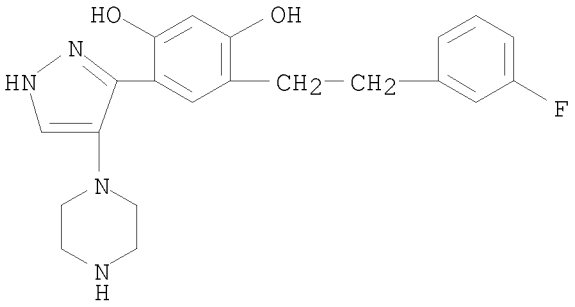
RN 719287-93-1 CAPLUS
CN 1,3-Benzenediol, 4-[2-(2,5-dimethoxyphenyl)ethyl]-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



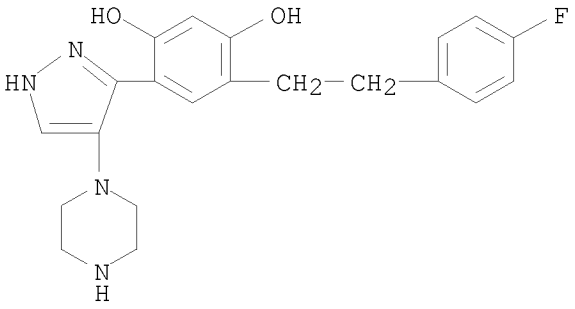
RN 719287-94-2 CAPLUS
CN 1,3-Benzenediol, 4-[2-(2-fluorophenyl)ethyl]-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



RN 719287-95-3 CAPLUS
CN 1,3-Benzenediol, 4-[2-(3-fluorophenyl)ethyl]-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

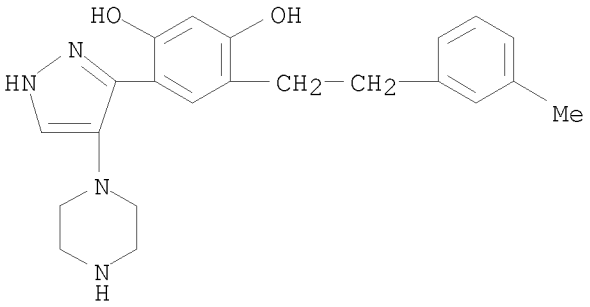


RN 719287-96-4 CAPLUS
CN 1,3-Benzenediol, 4-[2-(4-fluorophenyl)ethyl]-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

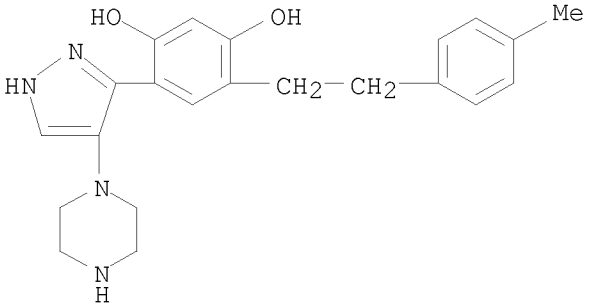


RN 719287-97-5 CAPLUS
CN 1,3-Benzenediol, 4-[2-(3-methylphenyl)ethyl]-6-[4-(1-piperazinyl)-1H-

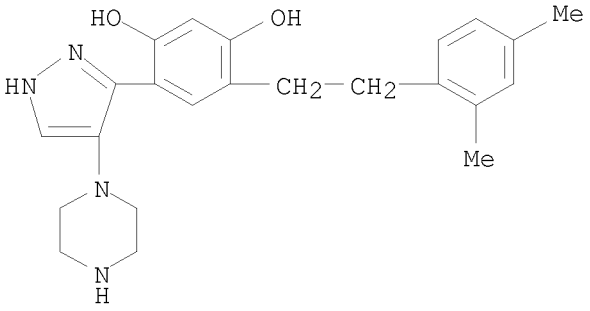
pyrazol-3-yl]- (CA INDEX NAME)



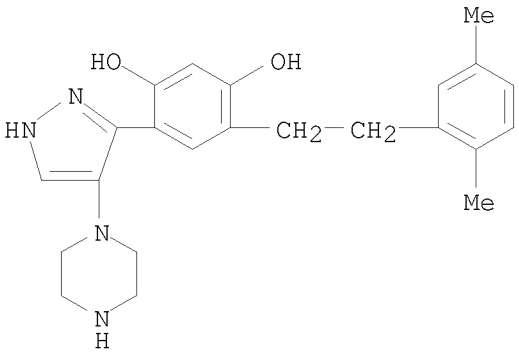
RN 719287-98-6 CAPLUS
CN 1,3-Benzenediol, 4-[2-(4-methylphenyl)ethyl]-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



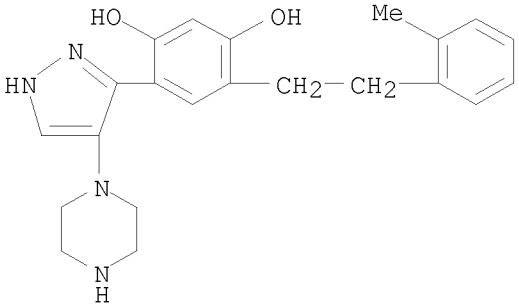
RN 719287-99-7 CAPLUS
CN 1,3-Benzenediol, 4-[2-(2,4-dimethylphenyl)ethyl]-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



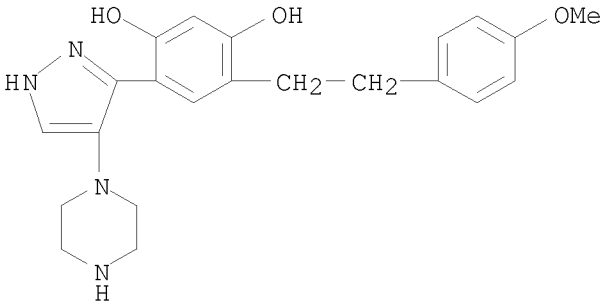
RN 719288-00-3 CAPLUS
CN 1,3-Benzenediol, 4-[2-(2,5-dimethylphenyl)ethyl]-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



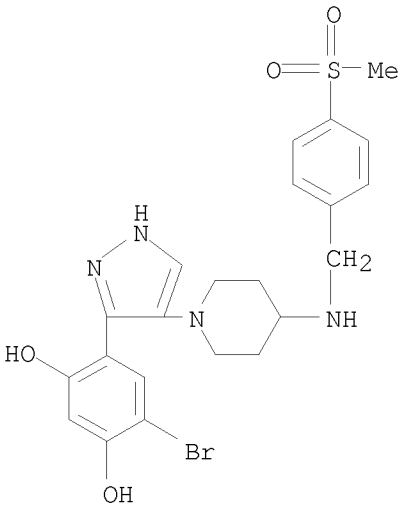
RN 719288-01-4 CAPLUS
CN 1,3-Benzenediol, 4-[2-(2-methylphenyl)ethyl]-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



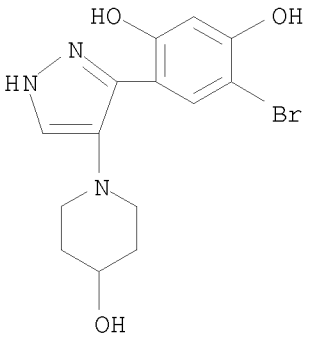
RN 719288-02-5 CAPLUS
CN 1,3-Benzenediol, 4-[2-(4-methoxyphenyl)ethyl]-6-[4-(1-piperazinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



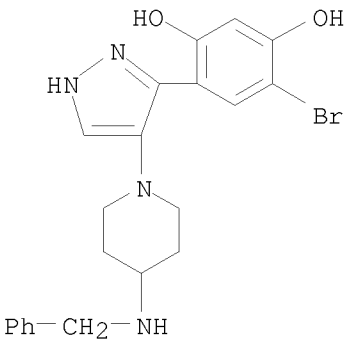
RN 719288-03-6 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-[4-[[[4-(methylsulfonyl)phenyl]methyl]amino]-1-piperidinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



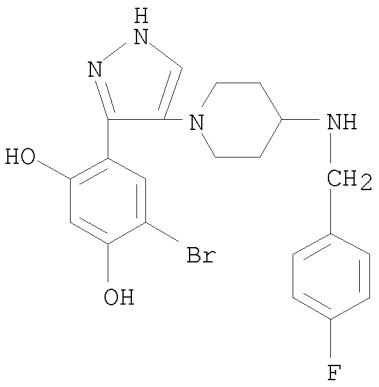
RN 719288-04-7 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-(4-hydroxy-1-piperidinyl)-1H-pyrazol-3-yl]-
(CA INDEX NAME)



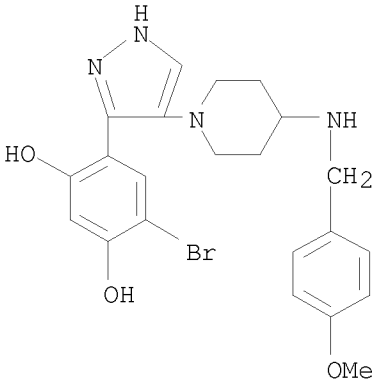
RN 719288-05-8 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-[4-[(phenylmethyl)amino]-1-piperidinyl]-1H-
pyrazol-3-yl]- (CA INDEX NAME)



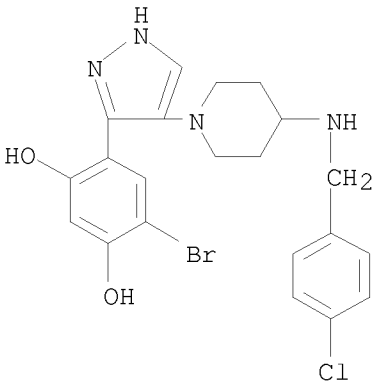
RN 719288-06-9 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-[4-[[(4-fluorophenyl)methyl]amino]-1-piperidinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



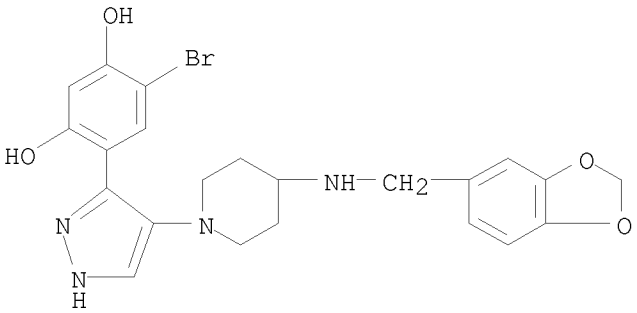
RN 719288-07-0 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-[4-[[(4-methoxyphenyl)methyl]amino]-1-piperidinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



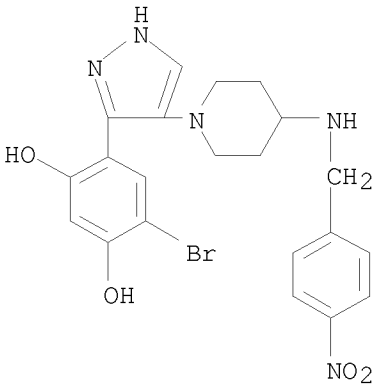
RN 719288-08-1 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-[4-[[(4-chlorophenyl)methyl]amino]-1-piperidinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



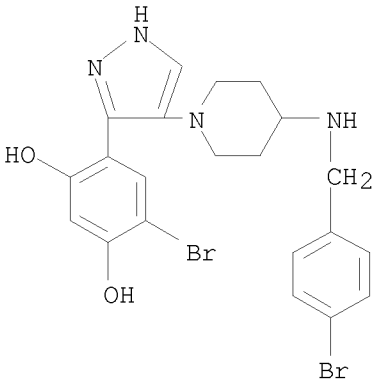
RN 719288-09-2 CAPLUS
CN 1,3-Benzenediol, 4-[4-[4-[(1,3-benzodioxol-5-ylmethyl)amino]-1-piperidinyl]-1H-pyrazol-3-yl]-6-bromo- (CA INDEX NAME)



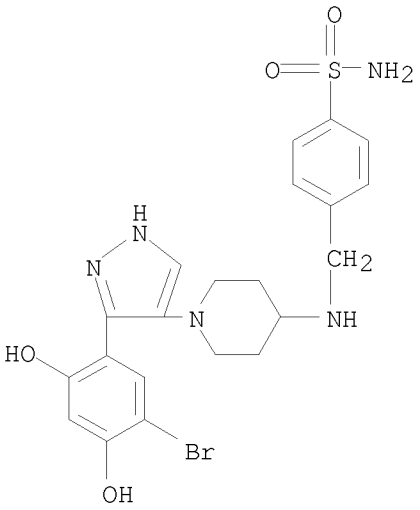
RN 719288-10-5 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-[4-[[(4-nitrophenyl)methyl]amino]-1-piperidinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



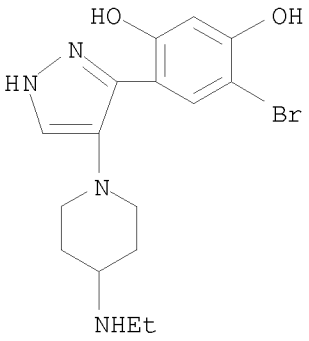
RN 719288-11-6 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-[4-[[(4-bromophenyl)methyl]amino]-1-piperidinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



RN 719288-12-7 CAPLUS
CN Benzenesulfonamide, 4-[[[1-[3-(5-bromo-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]-4-piperidinyl]amino]methyl]- (CA INDEX NAME)



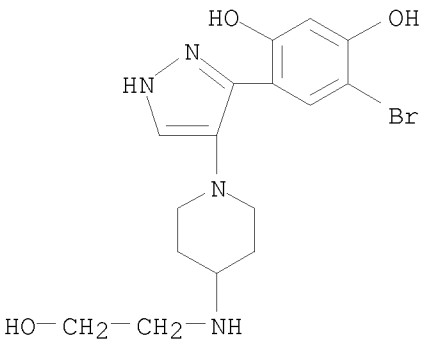
RN 719288-13-8 CAPLUS
CN 1,3-Benzenediol, 4-bromo-6-[4-[4-(ethylamino)-1-piperidinyl]-1H-pyrazol-3-yl]- (CA INDEX NAME)



RN 719288-15-0 CAPLUS
CN Formic acid, compd. with 4-bromo-6-[4-[4-[(2-hydroxyethyl)amino]-1-piperidinyl]-1H-pyrazol-3-yl]-1,3-benzenediol (1:1) (CA INDEX NAME)

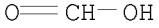
CM 1

CRN 719288-14-9
CMF C16 H21 Br N4 O3



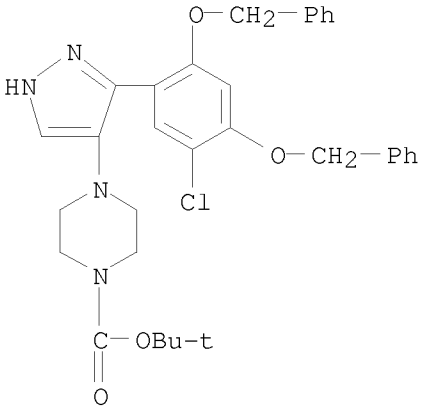
CM 2

CRN 64-18-6
CMF C H2 O2

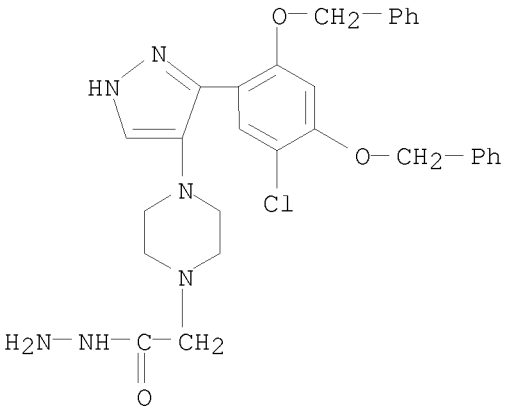


IT 719288-18-3P 719288-20-7P 719288-27-4P
719288-31-0P 719288-39-8P 719288-43-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazoles as inhibitors of HSP90)

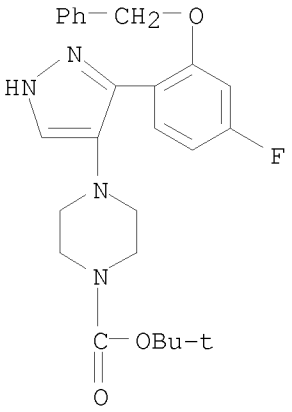
RN 719288-18-3 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[3-[5-chloro-2,4-bis(phenylmethoxy)phenyl]-1H-pyrazol-4-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



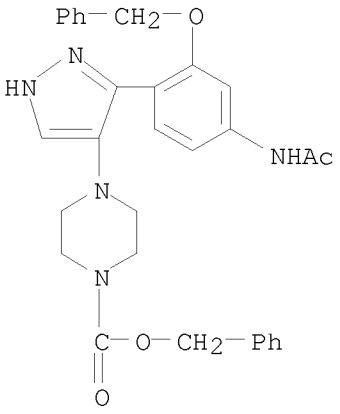
RN 719288-20-7 CAPLUS
CN 1-Piperazineacetic acid, 4-[3-[5-chloro-2,4-bis(phenylmethoxy)phenyl]-1H-pyrazol-4-yl]-, hydrazide (CA INDEX NAME)



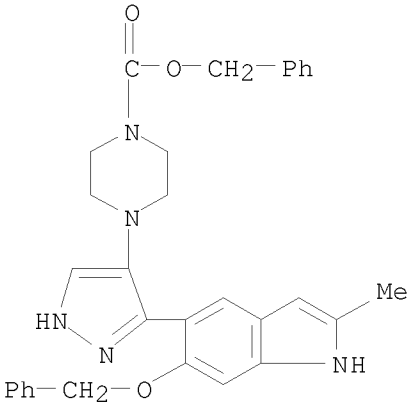
RN 719288-27-4 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[3-[4-fluoro-2-(phenylmethoxy)phenyl]-1H-pyrazol-4-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



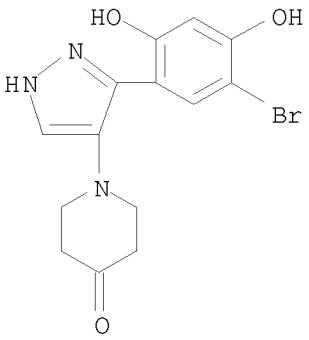
RN 719288-31-0 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[3-[4-(acetylamino)-2-(phenylmethoxy)phenyl]-1H-pyrazol-4-yl]-, phenylmethyl ester (CA INDEX NAME)



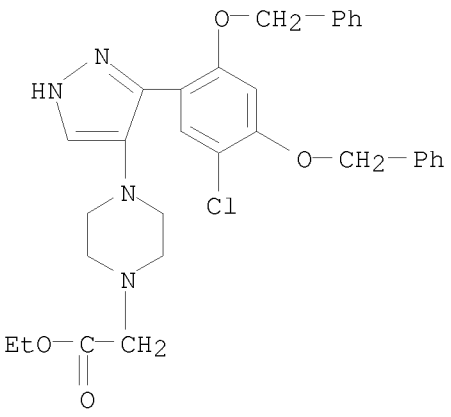
RN 719288-39-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[3-[2-methyl-6-(phenylmethoxy)-1H-indol-5-yl]-1H-pyrazol-4-yl]-, phenylmethyl ester (CA INDEX NAME)



RN 719288-43-4 CAPLUS
CN 4-Piperidinone, 1-[3-(5-bromo-2,4-dihydroxyphenyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)



IT 719288-21-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrazoles as inhibitors of HSP90)
RN 719288-21-8 CAPLUS
CN 1-Piperazineacetic acid, 4-[3-[5-chloro-2,4-bis(phenylmethoxy)phenyl]-1H-pyrazol-4-yl]-, ethyl ester (CA INDEX NAME)



RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1996:121332 CAPLUS
DN 124:289529
TI 3-[4-(Methylsulfonyl)phenyl]-1H-pyrazoles and 4-(1H-pyrazol-3-yl)benzenesulfonamides as selective inhibitors of cyclooxygenase II useful as inflammation inhibitors
IN Lee, Len F.; Penning, Thomas D.; Kramer, Steven W.
PA G. D. Searle and Co., USA
SO U.S., 40 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5486534	A	19960123	US 1994-278297	19940721
	CA 2195123	A1	19960208	CA 1995-2195123	19950720
	WO 9603385	A1	19960208	WO 1995-US8788	19950720
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
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	AU 9531267	A	19960222	AU 1995-31267	19950720
	EP 772597	A1	19970514	EP 1995-927154	19950720
	EP 772597	B1	20011212		
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	JP 10503201	T	19980324	JP 1996-505781	19950720

	JP 3490716	B2	20040126		
	EP 1127878	A1	20010829	EP 2001-112883	19950720
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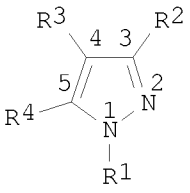
	AT 210648	T	20011215	AT 1995-927154	19950720
	PT 772597	T	20020531	PT 1995-927154	19950720
	ES 2169760	T3	20020716	ES 1995-927154	19950720
	US 5580985	A	19961203	US 1995-535688	19950928
	US 5756530	A	19980526	US 1996-721787	19960925
	US 6028072	A	20000222	US 1997-776090	19970609
PRAI	US 1994-278297	A	19940721		
	EP 1995-927154	A3	19950720		
	WO 1995-US8788	W	19950720		

OS CASREACT 124:289529; MARPAT 124:289529

GI



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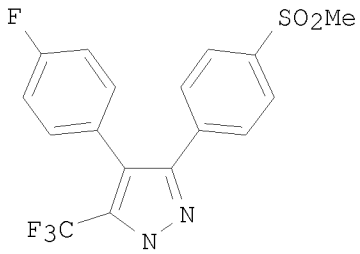
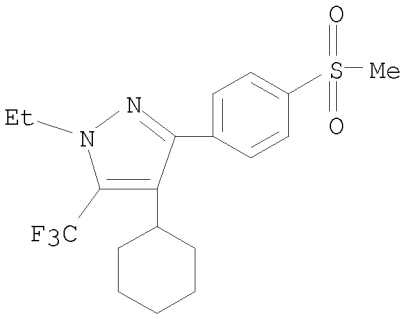


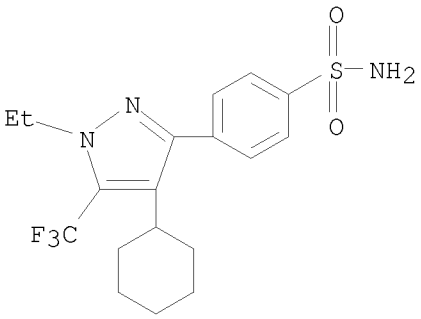
II

AB A class of pyrazolyl compds. is described for use in treating inflammation and inflammation-related disorders and is defined by formula I wherein R1 is a radical selected from hydrido, alkyl, alkenyl, alkynyl, haloalkyl, aralkyl, hydroxyalkyl, alkoxyalkyl, cyanoalkyl, aminoalkyl, alkylaminoalkyl, carboxyalkyl, alkoxycarbonylalkyl, alkylaminocarbonylalkyl, N-hydroxyaminocarbonylalkyl, N-hydroxy-N-alkyl-aminocarbonylalkyl, arylaminocarbonylalkyl and aminocarbonylalkyl; wherein R2 is aryl substituted at a substitutable position with a radical selected from alkylsulfonyl and sulfamyl; wherein R3 is selected from aryl, cycloalkyl, and cycloalkenyl; wherein R3 is optionally substituted at a substitutable position with one or more radicals selected from halo, alkylthio, alkylsulfinyl, alkyl, cyano, carboxyl, alkoxycarbonyl, aminocarbonyl, alkylaminocarbonyl, arylaminocarbonyl, N-alkyl-N-arylaminocarbonyl, haloalkyl, hydroxyl, alkoxy, hydroxyalkyl, haloalkoxy, amino, alkylamino, arylamino, heterocyclo and nitro; and wherein R4 is selected from hydrido, alkyl, haloalkyl, carboxyalkyl, alkoxycarbonylalkyl, aralkoxycarbonylalkyl, aminocarbonylalkyl, hydroxyalkyl and aralkoxyalkyl; or a pharmaceutically-acceptable salt thereof. Thus, e.g., acylation of thioanisole with 4-fluorophenylacetic acid afforded 2-(4-fluorophenyl)-1-[4-(methylthio)phenyl]ethanone; acylation of the latter with 1-trifluoroacetylimidazole followed by heterocyclization with hydrazine afforded 4-(4-fluorophenyl)-3-[4-(methylthio)phenyl]-5-(trifluoromethyl)-1H-pyrazole; oxidation of latter to the 4-methylsulfonyl derivative followed by 1-ethylation afforded 1-ethyl-4-(4-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-5-(trifluoromethyl)-1H-pyrazole (II) which exhibited selective inhibition of cyclooxygenase II: ID50 = >10 μM for COX I, and <0.1 μM for COX II.

IT 175678-37-2P 175679-99-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(3-[4-(methylsulfonyl)phenyl]-1H-pyrazoles and 4-(1H-pyrazol-3-yl)benzenesulfonamides as selective inhibitors of cyclooxygenase II useful as inflammation inhibitors)
RN 175678-37-2 CAPLUS
CN 1H-Pyrazole, 4-cyclohexyl-1-ethyl-3-[4-(methylsulfonyl)phenyl]-5-(trifluoromethyl)- (CA INDEX NAME)



RN 175679-99-9 CAPLUS
CN Benzenesulfonamide, 4-[4-cyclohexyl-1-ethyl-5-(trifluoromethyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)



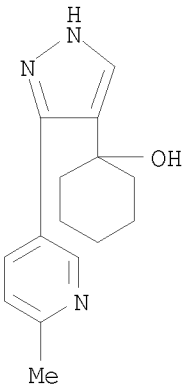
L14 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1970:445406 CAPLUS
DN 73:45406
OREF 73:7491a,7494a
TI Addition of diazomethane to β-ethynylpyridines
AU Terent'ev, P. B.; Moskvina, T. P.; Moshentseva, L. V.; Kost, A. N.
CS Mosk. Gos. Univ. im. Lomonosova, Moscow, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1970), (4), 498-502
CODEN: KGSSAQ; ISSN: 0132-6244
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB To a solution of EtMgBr (from 4.8 g Mg and 32.6 g EtBr) in 120 ml

tetrahydrofuran (THF) was added, during 1 hr, 23.4 g 2-methyl-5-ethynylpyridine (I) in 60 ml THF, and the mixture heated 20 min at 60-70° to yield 58% (2-methyl-5-pyridyl)propiolic acid (II), ml. 231-2°. To 55 g I was added dropwise 60 ml 27.5% H2O2, 51 ml Ac2O was added so as to keep the temperature at 60-70°, the mixture kept 2 hr at 60-5°, 2 ml 40% formalin added, and heating continued 1 hr to yield 64% I 1-oxide (III), m. 158-60° (Me2CO). To 1.33 g III in 10 ml Me2SO was added CH2N2 [from 30 g nitrosomethylurea (IV)] in 300 ml Et2O and the mixture kept in the dark 6 days at room temperature to yield 1.7 g V (R = Me) 1-oxide (VI), m. 241° (EtOH). To 3.5 g I in 10 ml Et2O was added CH2N2 (from 60 g IV) in 600 ml Et2O and the mixture kept 3 days in the dark to yield 41% V (R = Me) (VII, m. 123-4° (C6H6). To 0.35 g VI in 20 ml CHCl3 was added, at 0°, 1 g PCl3 and the mixture heated 1 hr at 70-80° to yield 64% VII. To 1 g VII in 30 ml Me2SO was added 1.11 g SeO2 and the mixture heated 20 min at 110-20°, and at the end 140-50°, to yield 23% V (R = CO2H) (VIII), m. 250-60° (decompn). VIII was decarboxylated by heating in vacuo at 250-70° to yield V (R = H); picrate m. 194-6° (EtOH). To 0.01 mole 2-methyl-5-(2-R-substituted-ethynyl)pyridine in Et2O was added CH2N2 (from 20 g IV) in 200 ml Et2O and the mixture kept 10 days in the dark to yield IX (R, m.p., m.p. picrate, and % yield given): 1-hydroxycyclohexyl, 150-1° (petroleum ether) -, 16; morpholinomethyl, 145-6° (hexane), -, 28; Et2N, -, 158-9° (EtOH), 10; To 4.83 g II in 60 ml Me2SO was added CH2N2 (from 100 g IV) in 1 l. Et2O and the mixture kept 6 days at room temperature in the dark to yield 12% X (R = CO2Me), m. 85-6°, and 20% XI, (R = CO2Me); picrate m. 155°. A mixture of 0.3 g X (R = CO2Me) and 20 ml 2M NaOH refluxed 20 min gave 89% X (R = CO2H), m. 160-1°, which, after decarboxylation at 200° in vacuo, gave X (R = H); picrate m. 227-8° (EtOH). Similarly, 6-hr reflux gave 88% XI (R = CO2H), m. 258-60° (EtOH), which, decarboxylated at 250-70° in vacuo, afforded XI (R = H); picrate m. 242-3° (EtOH). To 1.47 g 5-ethylpicolinic acid in 20 ml Et2O was added 200 ml Et2O containing CH2N2 (from 30 g IV) and the mixture kept 6 days at room temperature in the dark to yield 39% XII, m. 145-6°.

IT 27509-32-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 27509-32-6 CAPLUS

CN Cyclohexanol, 1-[3-(6-methyl-3-pyridyl)pyrazol-4-yl]- (8CI) (CA INDEX NAME)

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